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Web: www.genesis-tutorials.com
Email: info@genesis-tutorials.com
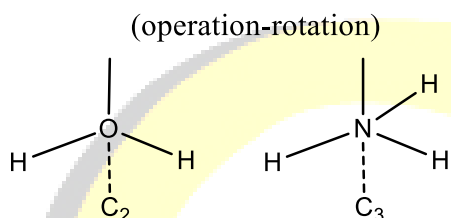
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Stereochemistry

Elements of symmetry:-

(1) Axis of symmetry:- (Cn)→ Imaginary axis passes through the centre of the molecule called axis of symmetry, highest order of the axis of symmetry called principle axis, remaining axis is subsidiary axis.

Example:-

(operation-rotation)

(2) Plane of symmetry:- (σ) → Any molecule having 3 types of possible plane—

(1) σ_v – vertical plane– plane parallel to principle axis.

(2) σ_h – Horizontal plane or molecular plane.

(3) σ_d – Dihydral plane (operation reflexion).

σ_h – plane perpendicular to principle axis.

σ_d – place bisect two C_z angle.

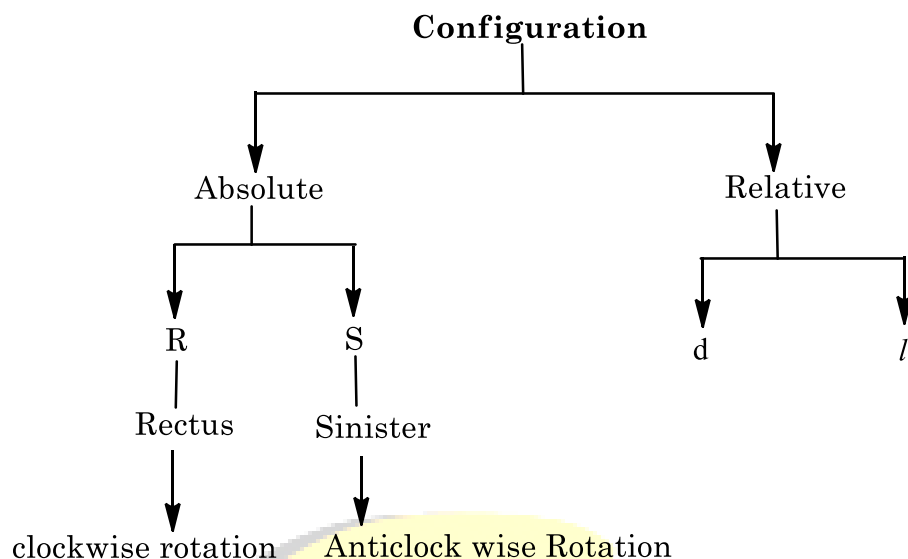**(3) Inversion centre (centre of symmetry)**:- (i) operation–inversion

Note:- i present → optically inactive compound

A centre of symmetry is a point with in a molecule such that if an atom is joint to it and the line plotted to an equal distance beyond, it incounters an equivalent atoms or point.

(4) Improper axis of symmetry (Sn):- (Operation – Roto-reflexion)

Rotation followed by reflexion in a plane perpendicular to the axis generate a structure indistinguishable from the original.

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(5) Indentity (ε) – (operation-nothing to do)

Configuration

- Absolute
  - R — Rectus → clockwise rotation
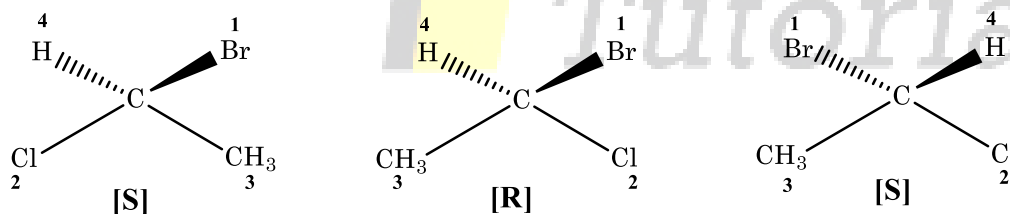 - S — Sinister → Anticlock wise Rotation
- Relative
  - d
  - l

* CIP Rules:- (Cahn-Inglod-Prelog):-

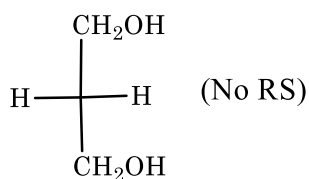**Order of priority**– I > Br > Cl > F (On the basis of atomic number)

Assign priority of the different substituents accordingly.

(i) Lowest priority group must away from observer.

(ii) Rotates the eye with decreasing order of priority.

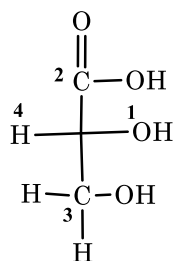(iii) Priority gives according to atomic number but in case of isotopes priority assign on the basis of atomic mass.
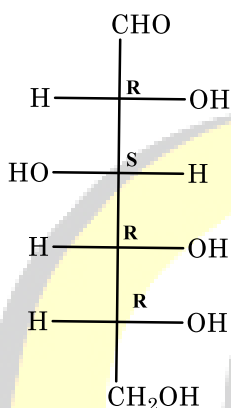

(Wedge-Dash representation) - [3D]

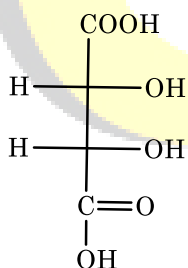**Note**:- RS nomenclature always gives chiral molecule

(No RS)

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Fisher representation:- (2-D) [R]

$$
\begin{array}{c}
\overset{O}{\underset{\parallel}{}} \\
^{2}\,C\text{—OH} \\
^{4}H\text{—}\!\!\overset{1}{\underset{}{\underset{|}{}}}\text{—OH} \\
H\text{—}\underset{3}{C}\text{—OH} \\
|\\
H
\end{array}
$$

In case of carbohydrate, if the OH group will be right then configuration is [R] and OH is in left then [S].

$$
\begin{array}{c}
CHO \\
H\text{—}\overset{R}{|}\text{—OH} \\
HO\text{—}\overset{S}{|}\text{—H} \\
H\text{—}\overset{R}{|}\text{—OH} \\
H\text{—}\overset{R}{|}\text{—OH} \\
CH_2OH
\end{array}
$$
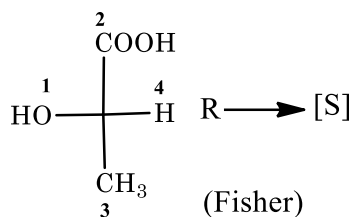
* Mesotartic acid is optically inactive due to internal compensation

$$
\begin{array}{c}
COOH \\
H\text{—}|\text{—OH} \\
H\text{—}|\text{—OH} \\
C\!\!=\!\!O \\
|\\
OH
\end{array}
$$

(1)

$$
\begin{array}{c}
^{3}CH_3 \\
\end{array}
\qquad \equiv \qquad
\begin{array}{c}
COOH \\
H\text{—}|\text{—OH} \\
CH_3
\end{array}
$$

[R]   (Latic acid)

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(2)

(Fisher) → [S]

(3)

O > M > P
(priority order)

[R]
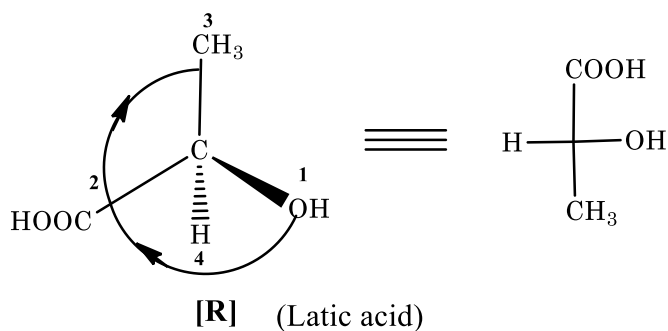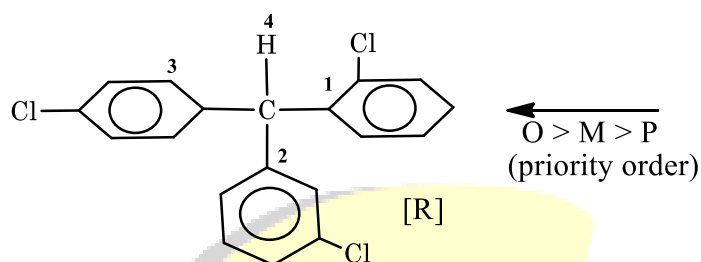
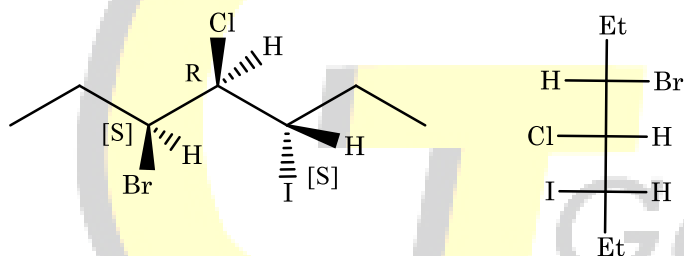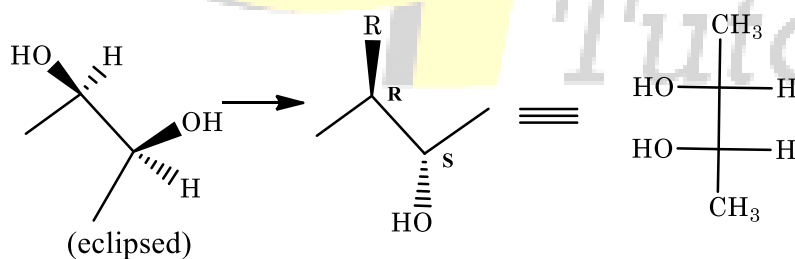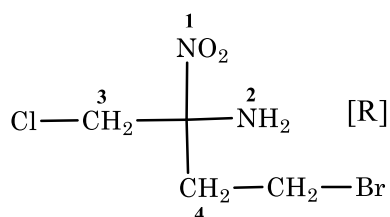**(4)**

(5) Note:- Fisher representation always show eclipsed form.

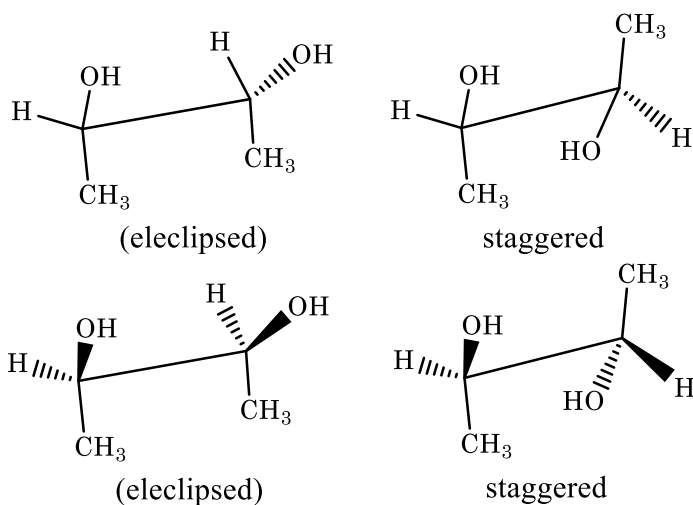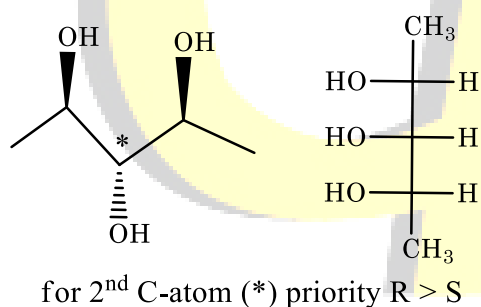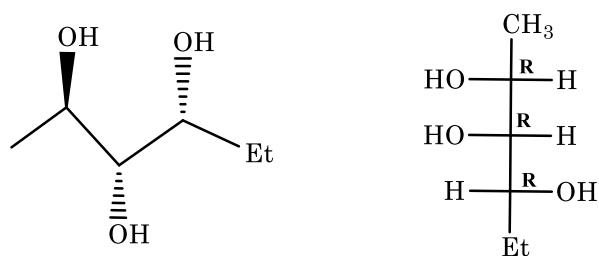(eclipsed)

(6)

[R]

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(7)

$$
\begin{array}{c}
CH_2OH \\
| \\
C=O \\
| \\
HO-C-H \\
| \\
H-C-OH \\
| \\
H-C-OH \\
| \\
CH_2OH
\end{array}
\qquad (Fructose)
$$

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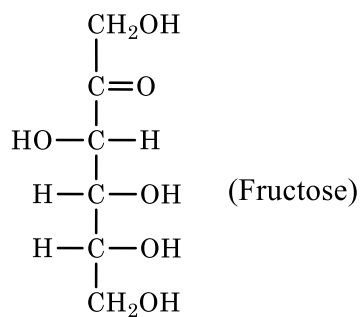
* Saw-horse projection formula

(eleclipsed)   staggered

(eleclipsed)   staggered

(1)

for 2nd C-atom (*) priority R > S

(2)

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* Relative configurations:-

(1)

```
        CHO                          CHO
         |                            |
  H ─────┼───── OH          HO ───────┼───── H
         |                            |
       CH₂OH                        CH₂OH
  [D]-glyceraldehyde          [L-glyceraldehyde]
```

$$\text{[D]-glyceraldehyde} \quad\vdots\quad \text{[L-glyceraldehyde]}$$

(2)

```
        CH₃                          CH₃
         |                            |
  H ─────┼───── NH₂        H₂N ───────┼───── H
         |                            |
        COOH                         COOH
        [D]                          [L]
```
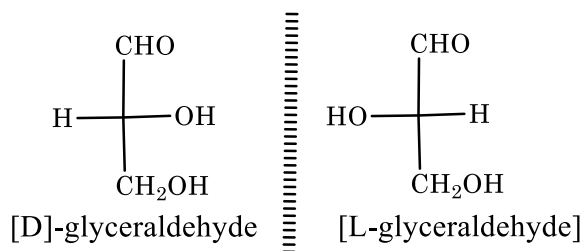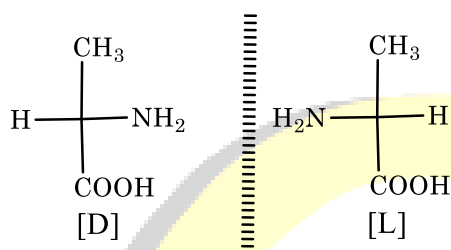
Serine is the standard of amine which is—

```
      CH₂─OH                       CH₂─OH
         |                            |
  H ─────┼───── NH₂        H₂N ───────┼───── H
         |                            |
        COOH                         COOH
     [D]-serine                      [L]
```
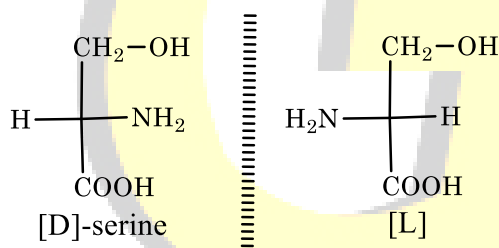
→ All amino acids having S configuration except cystein

→ Generally relative configuration used in carbohydrates and amino acids

Optical Activity: **The compounds having the ability to rotate the plane of polarized light (PPL) are called optically active (Chiral) compounds. This phenomenon is known as Optical Activity (Chirality)**

 * **CHIRALITY**

   Types of Chirality

   → centre of chirality

   → Axis of chirality (Axial chirality)

   → Plane of chirality

   → Halical chirality

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(i) Axial chirality:- Axial chirality show following compounds— **[ABS]**

    (i) Allenes

    (ii) Biphenyls

    (iii) Spyraives (spiranes)

Allenes:- $H_2C = C = CH_2$

          $CH_2 = CH - CH = CH_2$ — conjugated

          $CH_2 = CH - CH_2 - CH_2 - CH - CH_3$ — Isolated

          $HC = C = CH$ — Commulatated doublebond

Allene having cumulated double bond

Structure of Allenes:-

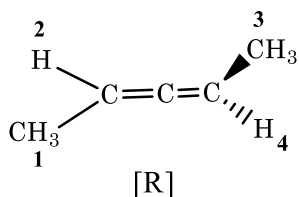If number of double bonds (2,4,6,8) (even) than terminal bond are present in the perpendicular plane.
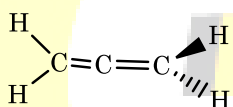
Odd number of double bonds (1,3,5,7) then terminal bonds are perpendicular to the plane present in same.
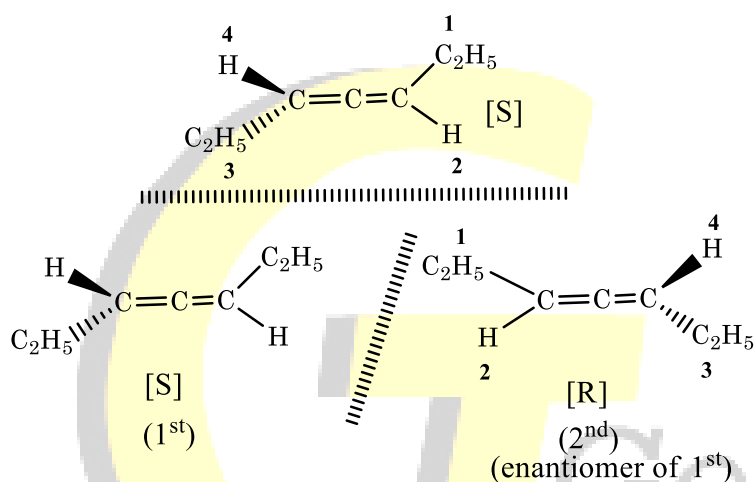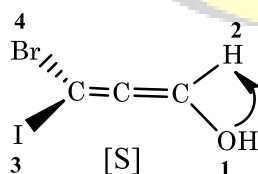

(point group P_2Cl)

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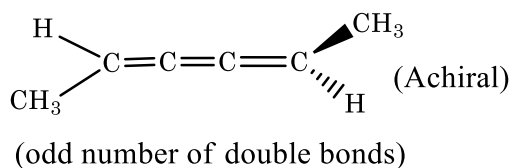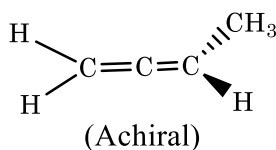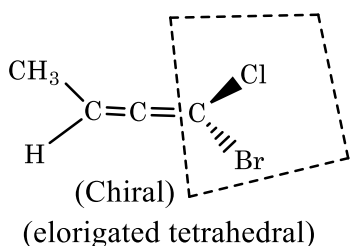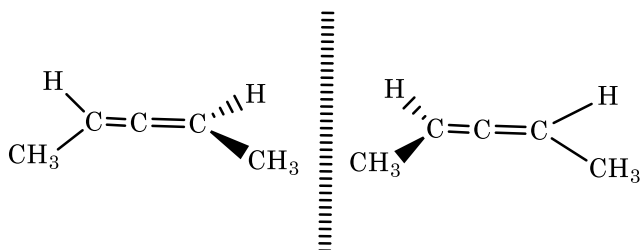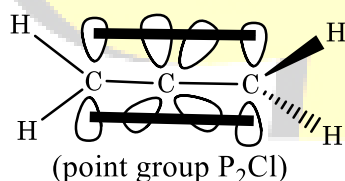
R/S nomenclature in Allene:-

(1)
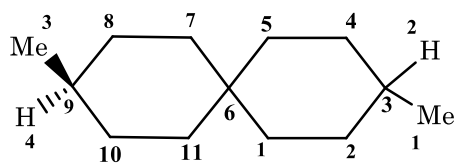

[R]

Trick- number start from in plane side group.

(2)

[S]

[S]
(1st)

[R]
(2nd)
(enantiomer of 1st)

(3)

[S]

* Spiranes:- Derivative of Allene

(Allene)   (Hemis-spirenes)   (spiranes)
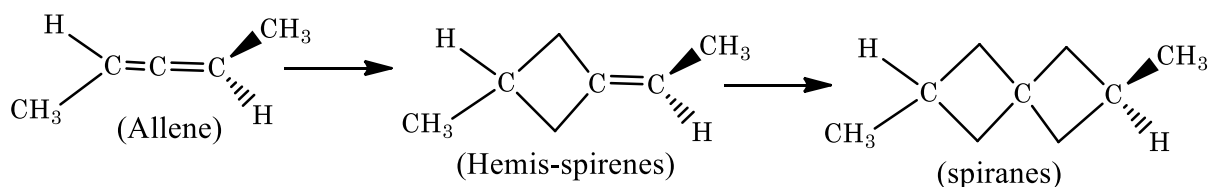
Note:-

This type of molecule doe not show axial chirality because terminal carbon not lie in C_z axis

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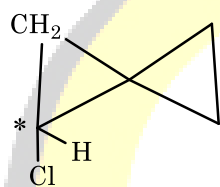**Email**: info@genesis-tutorials.com

[S]
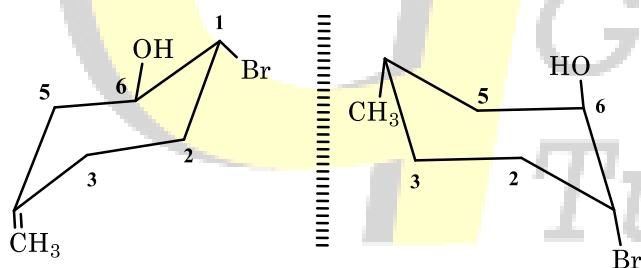3,9-dimethyl spiro [5,5,0]
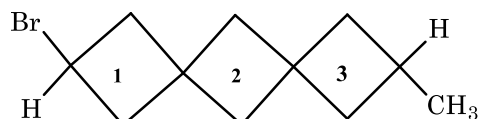
(Achiral)   (odd number of rings)

(due to σ-plane)

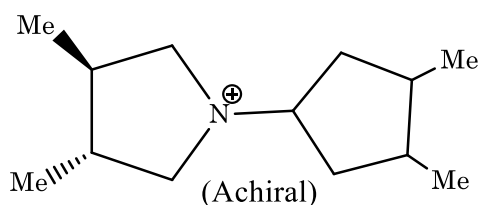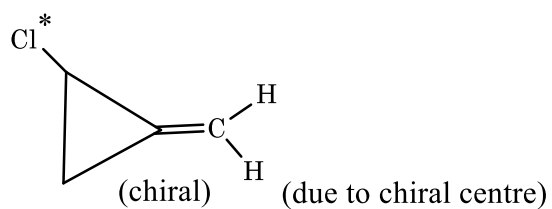## *Central Chirality in spiranes:- Chiral due or chiral centre

Example-1

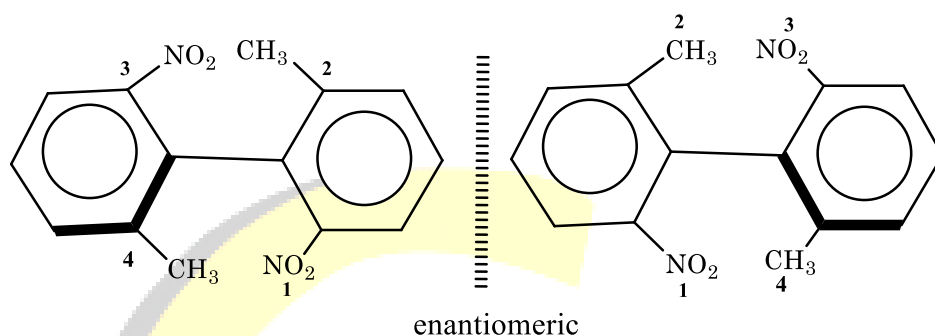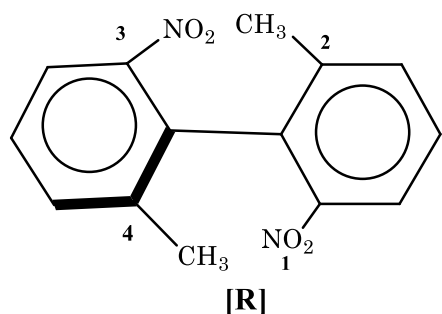## Example-2

Example-3

(Achiral)

Example-4

(chiral)   (due to chiral centre)

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BIPHENYLS:-

[R]

enantiomeric

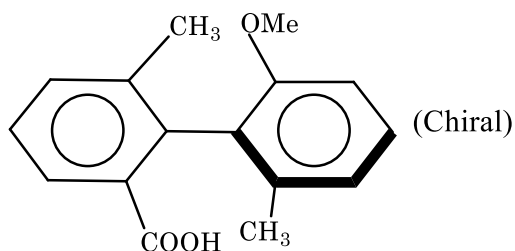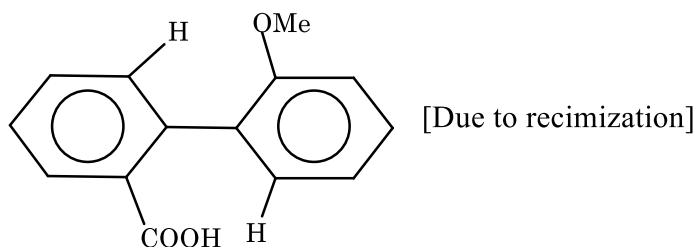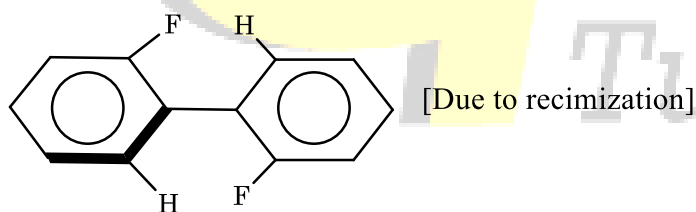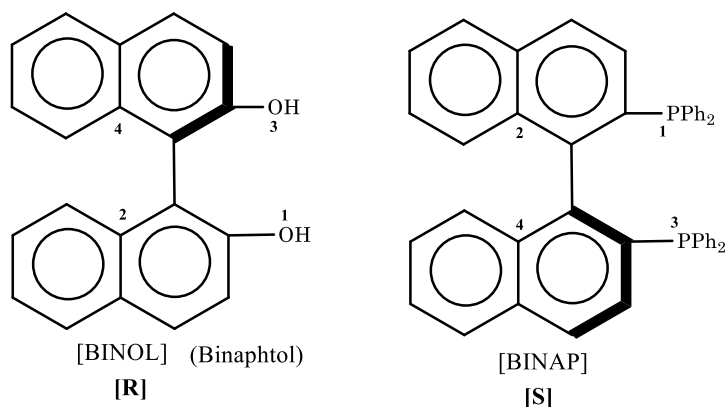## Essential conditions for chirality of biphenyls:-

(1) Proper substitution i.e. both ortho position of each benzene ring must have 2 different ligands.

(2) Ristriction of rotation or stable configuration that is O-substituent must be bulkyl group which is restricted rotation.

[Due to recimization]

[Due to recimization]

(Chiral)

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[BINOL] (Binaphtol)
**[R]**

[BINAP]
[S]

Note:- **Butteressing effect**

It has been found that if a substituent present at m-position of benzene ring in biphenyl the energy pf activation for recimization is enhance this is know as bulteresing effect of m-group.

It is due to ocetword bonding of ortho substituent by m-due to steric reason.

Bultersing effect increase with increasing of the size m substituent.
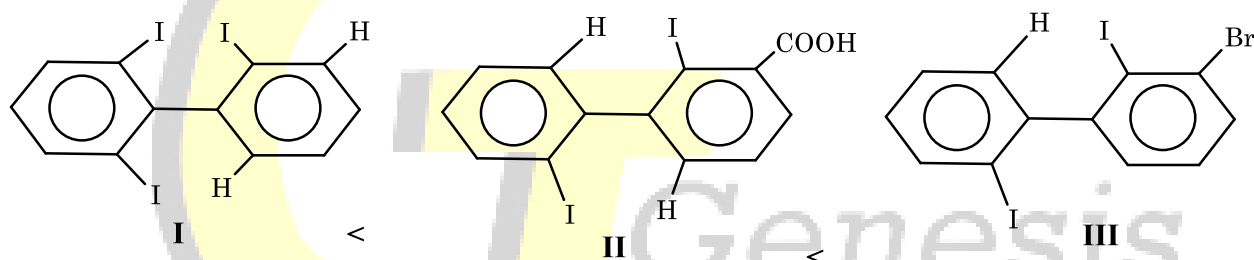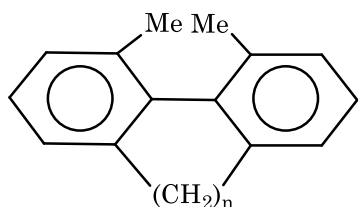

I   <   **II**   <   **III**

I < II < III (order of activation)
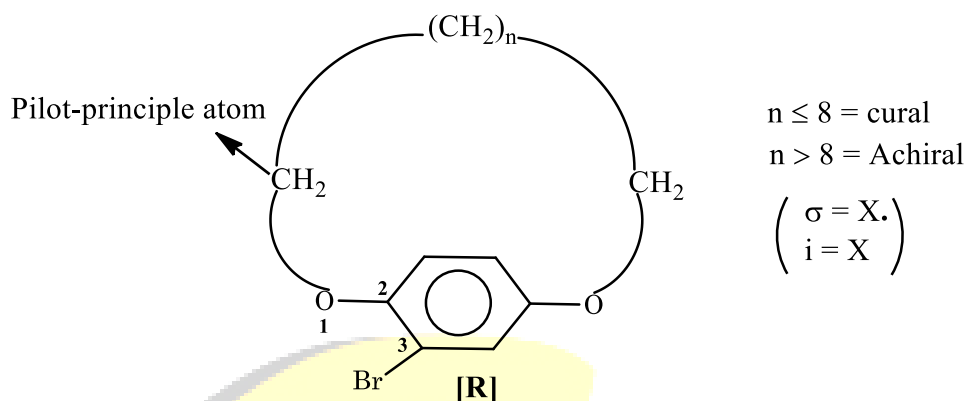
Br > Me > Cl > NO$_2$> COOH > F > H

Bultersing order(m-substituent)

Briged Biphenyls:-

if n = 1 – achiral due to r-plane

if n = 2,3 — chiral

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* **Atropisomerism**:- A molecule which is chiral due to oispictiction of rotation rivotal bond is known as atropisomer and this phenomenon is known as atropisomerism.

* **Chiral due to chiral plane**:-

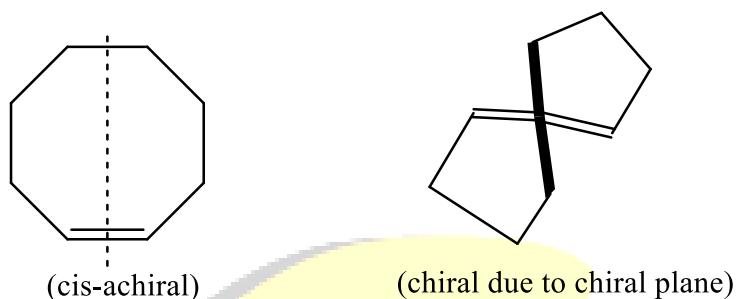**(1) Ansa-compounds:-**

$n \leq 8 =$ cural
$n > 8 =$ Achiral

$$\left(\begin{array}{l} \sigma = X. \\ i = X \end{array} \right)$$

(2) Paracyclophane:-

(Achiral)

pilotatom

[S]

(Achiral)

(chiral)

If n = 2, 3-chiral 3 > n
3 < n - Achiral

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(Ribox)

$$\left(\begin{array}{l} \text{left } \uparrow \\ \text{Right} \downarrow \end{array} \right)$$

(3) Trans-cyclootences:-

(cis-achiral)   (chiral due to chiral plane)
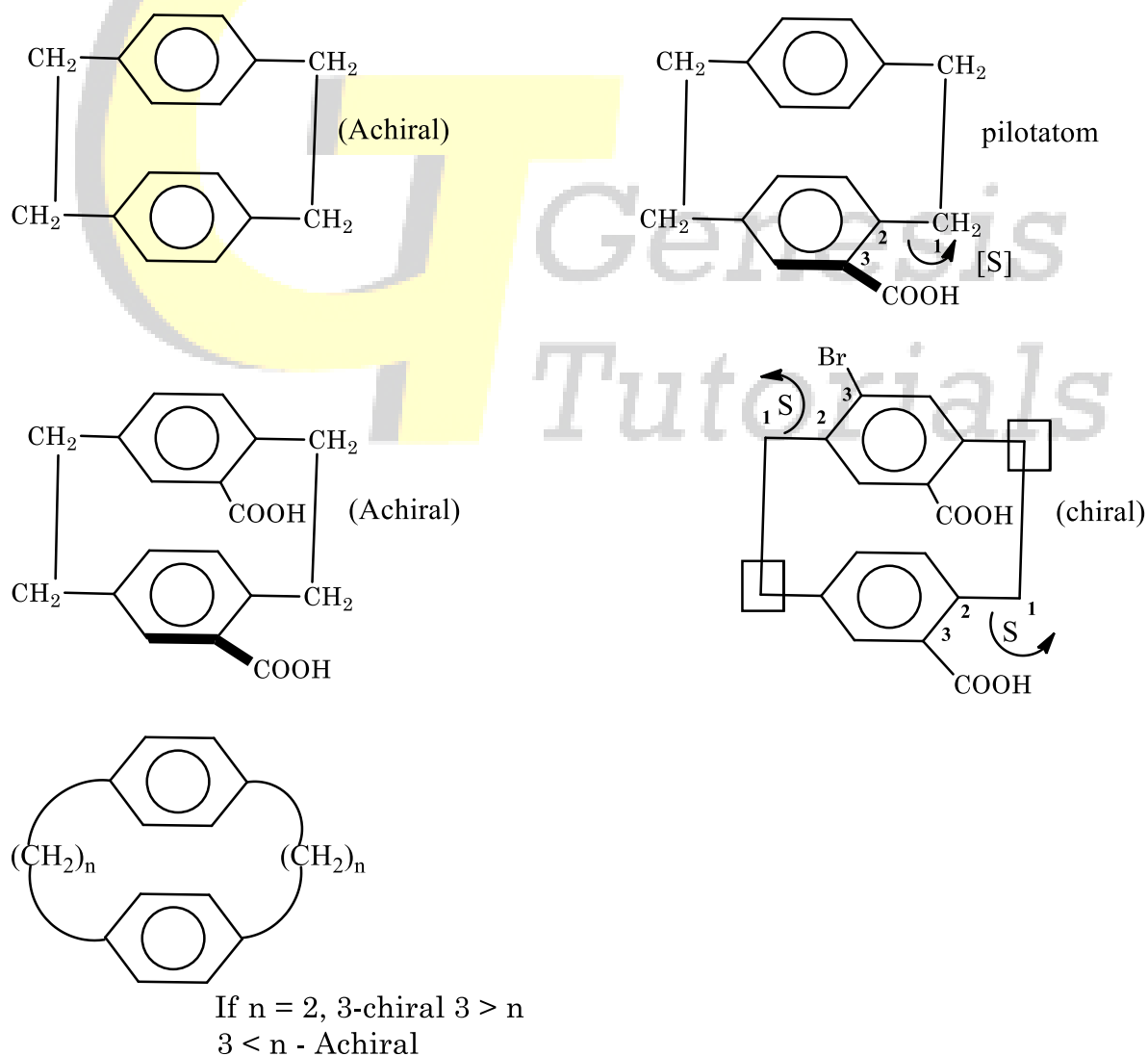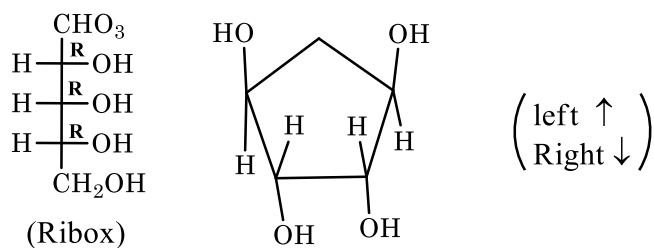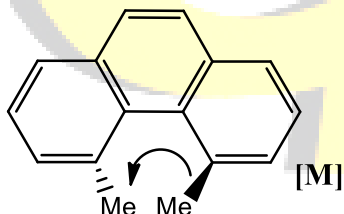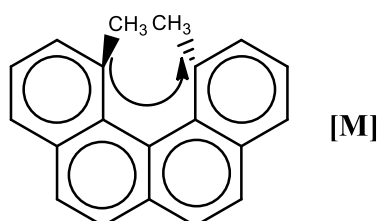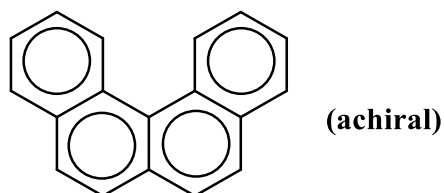
(4) Helicity:-

(i) For Helicity compound have minimum six ring

(ii) For helicity if the substituent are present then minimum have 3 in angular fashion.

P(+) → Clockwise

M(-) → Anti cloclwise

[M]

Note:- For prediction of P/M i.e. configuration in hedical structure, we strict from above to below [M].

(achiral)

[M]

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* Organometallic compounds

Example-1.

Staggeral
D_5d

eleclipse
D_5h
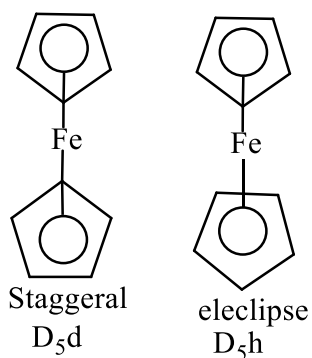
Example-2.
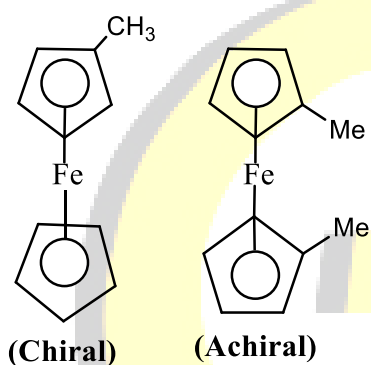
(Chiral)

(Achiral)

Example-3.
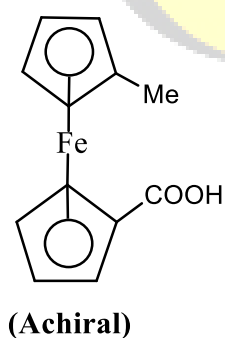
only 1 substituents are present in each ring that it will be achiral

(Achiral)

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Types of Stereoisomers:-

(1) Stereochemical Relation:-

(a) Enantiomers (Relative)

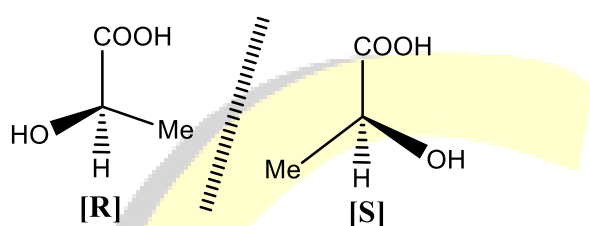**(b)** Diastoreomers (Relative)

(c) Meso compounds

(a) Enantiomers (Relative):- Those molecules which are non-superimpose mirror image with each other are known as enantiomer & this property is known enantiomers.

Note:- Enantiomers are always chiral molecules:-
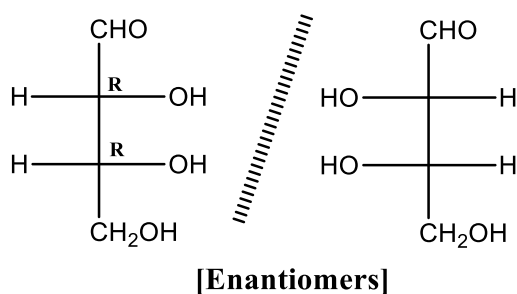

How to identity enantiomers?

(i) On the basis of mirror image:-

(ii) R/S nomerclature.

	No of Chiral centre	Molecule (A)	Molecule (B)
(a)	One	R	S
(b)	Two	R, R, Or S, S, R, S, S, R	S, S Or R, R, S, R, R, S
(c)	three	R, R, R, S, S, S, RSR so on	S,S,S R,R,R SRS so on

Example:-

[Enantiomers]

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(1)
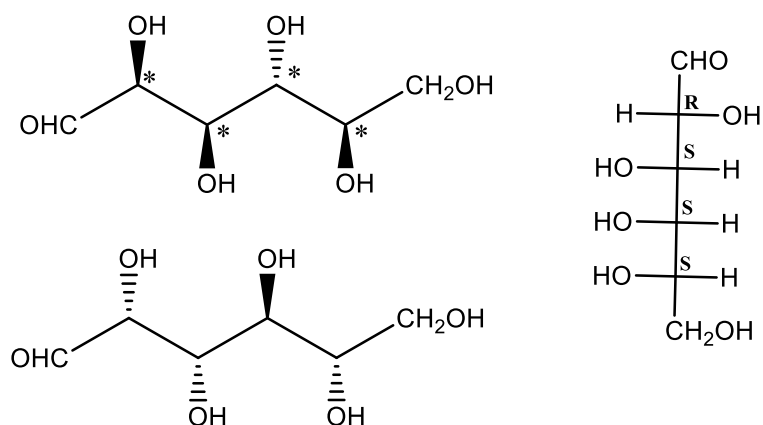
Note:-

[Enantiomers]
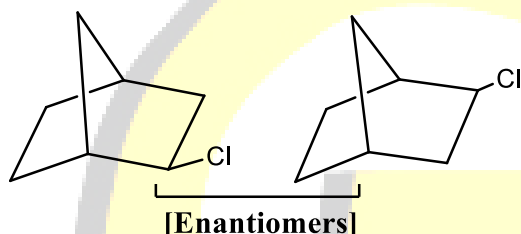
* exo-exo — enantiomer

* endo-endo — enantiomer

* **Propertied of enantiomers**:-

(1) They have same physical properties such as melting point, boiling point density refractive index, but they show different behaviour towards plan polarized light.

(2) They rotate parallel to opposite direction bur in equal magnitude.

A = $[\alpha]$ = -20°

B = $[\alpha]$ = +20°

(3) The isomer which rotate parallel in clockwise direction called dextro rotatry (d, (+)) and the isomer which rotate parallel anti clockwise rotation called levorotatory ((-), l).

(4) They have same chemical properties in achiral medium but they have different chemical properties in chiral medium.

(5) They have different playsilogical properties, Example:-

(-) nicotin is more possisonueous then (+) nicotin

(+) Histidine more surety

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(-) Histidine tastless

(+) Limonene- orange smell

(-) Limonene – Lemon smell

Enantiomers can't be distinguished by H-NMR system in achiral medium (solvent) but they can be distinguised in chiral medium.

* **Resolution**:- Separation of enantiomers from its recimic mixture is known as resolution.

* **Diatereomers:-** Those molecule which are not mirror image of each other is called diastereomers. They may or may not be chiral that is may or may not be optically active. Cis trans & E/Z nomenclature are always diastoreomers.

* How to identify?

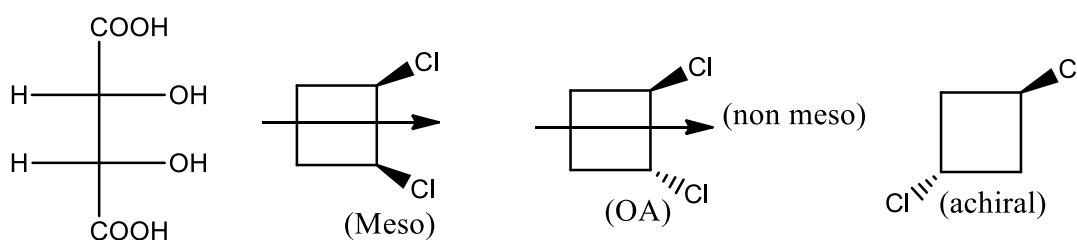| No of centre	A	B
1	R	S → No vesbe diastereomers.
2	RR	RS → diastereomers
3	RSS	RSR → diastereomers.
	RRR	SSR → [D]

Note:-

Exo-endo ⎤ Distereomers

Endo-exo ⎦
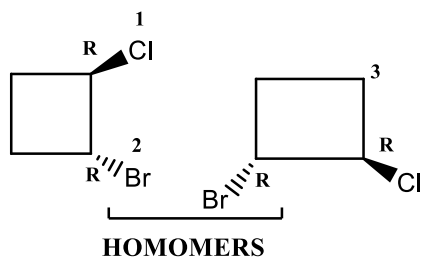

RRS

three chiral centre

SRS
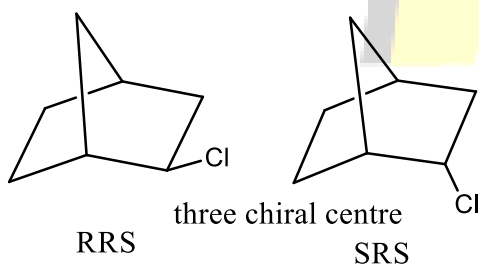
Meso compounds:- Compounds having more than 1 chiral centre but optically inactive due to presence of plane of symmetry are inversion centre are known as meso compounds.

Meso compounds are optically inactive due to internal compensation.

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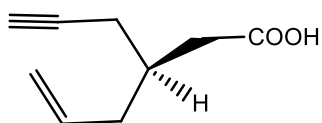
Homomers:- Homomers are identical with each other
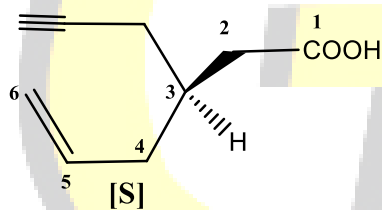

HOMOMERS

Question:-The IUPAC name of the following compound is   **[NET Dec 2011]**
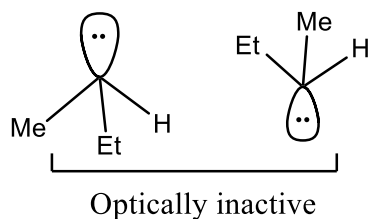

(a) (R)-3-(prop-2-enyl)hex-5-ynoic acid   (b) (S)-3-(prop-2-enyl)hex-5-ynoic acid

(c) (R)-3-(prop-2-enyl)hex-5-enoic acid   (d) (S)-3-(prop-2-ynyl)hex-5-enoic acid

Solution

(S)-3-(prop-2-enyl)hex-5-ynoic acid

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UMBRELLA INVERSION [NITROGEN INVERSION] OR PYRAMIDAL INVERSION

Optically inactive

N having trivalent (three group are different) and lone pair should be optically active but due to umberalla inversion or pyramidal inversion it becomes optically inactive (Recemization takes place)

But N having four different group it will be chiral

Optically active

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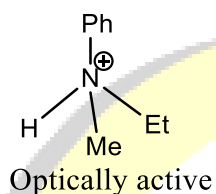
Prochirality and Topicity

* Prochirality:-

Prochiral centre:- A centre at which a single substitution makes centre chirality called prochiral centre.
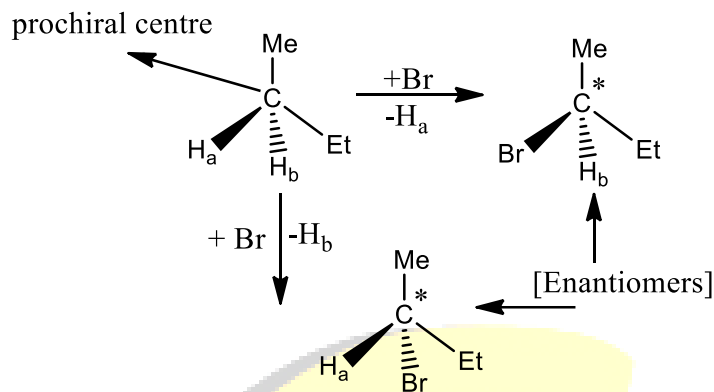
* **Pro stereogenic centre**:- A centre at which a single substitution by a new ligand gives a new stereogenic centre called pro stereogenic centre.
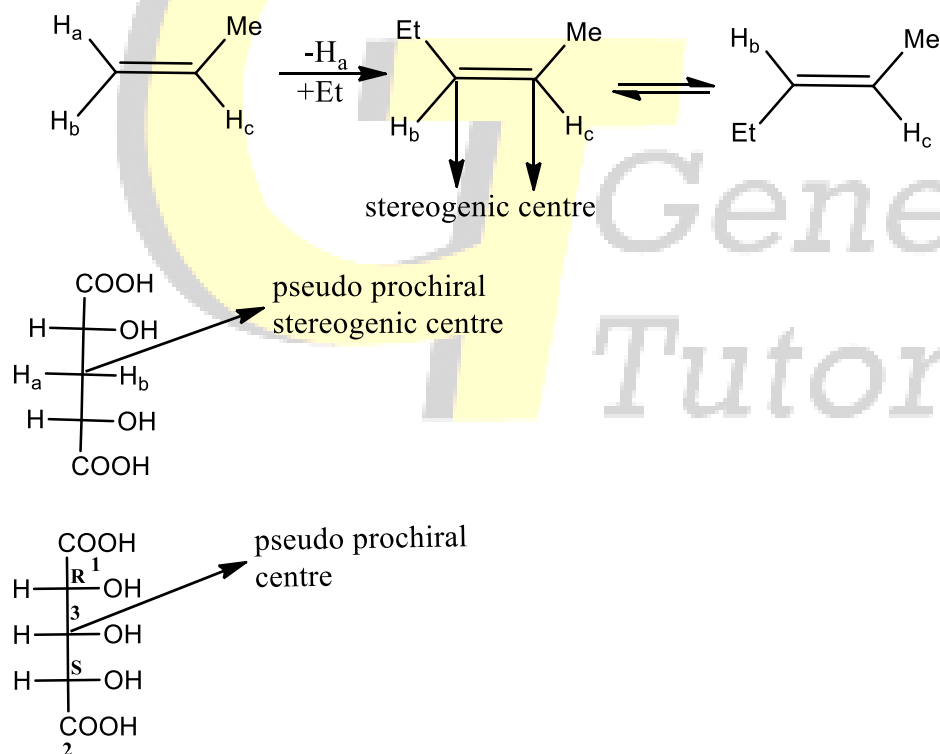
In pseudochiral centre, higher priority goes to R configuration

TOPICITY:- Stereo chemical relationship between two or more ligand within a molecule is defined in terms of topicity.

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Stereogenic centre:- A stereogenic centre is like a umbrella term under which a chiral centre is defined. A stereogenic centre is just a location in a molecule where the interchange of any two group gives a new stereoisomers.

On the basis of stereochemical relationship ligands of phases are classified in the following ways.

(i) Homotopic ligand

(ii) Hetrotopic ligand

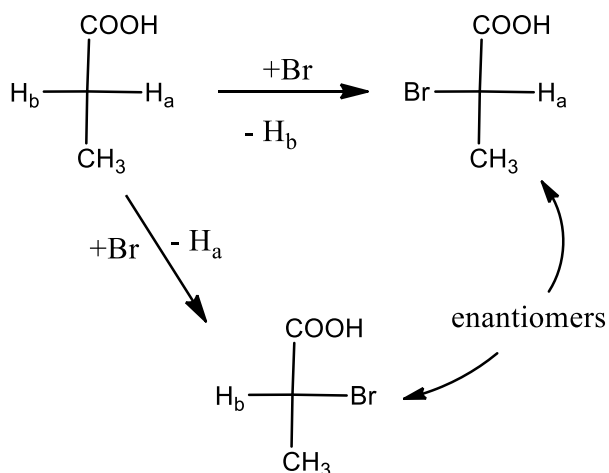(iii) Distereotopic ligand

(1) Homotopic ligand:- Two ligand are said to be homotopic if they are replaces by new ligand (achiral) gives a pair of two products which are identical or homomers to each other.
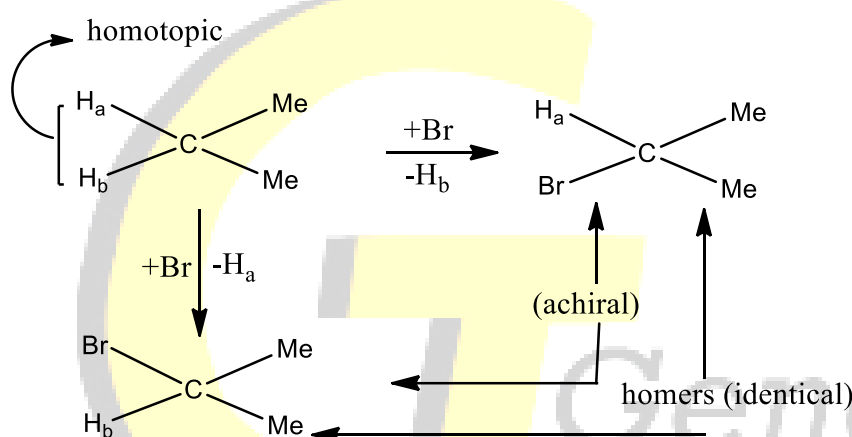
(2) Hetrotopic ligand

Two ligands are said to be hetrotopic if they are replaced by in turn by new ligands (chiral) gives two enantiomers

Hetrotopic ligands also called enantotopic ligands.

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(iii)Diastriotopic ligands:- Diastriotopic ligands ate not symmetry element C_n, I, S_n absent.

Compounds having diastriotopic ligands may or may not be chiral in the case of geometrical isomerism (achiral) but optical compounds are optically active.

Note:- Geometrical isomers (cis-tran/E-Z) are always diastereoromers with each optically inactive.
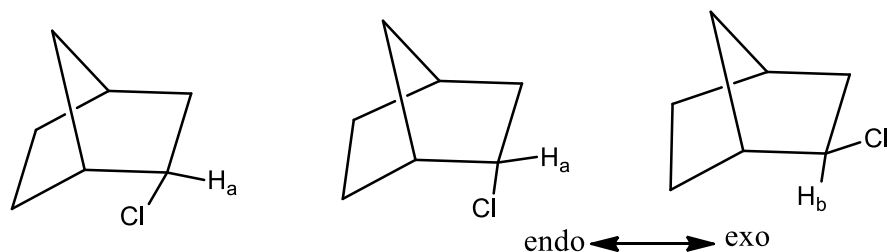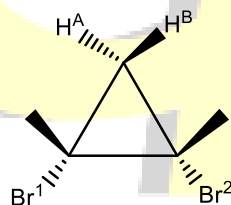

Question. The first person to separate a racemic mixture into individual enantiomers is

    (a) J, H van't Hoff   (b) Pasteur

    (c) H.E.Fischer   (d) F. Wohler   **[NET Dec 2012]**

Solution (b) Pasteur

Question. In the gcompound given below, the realtion between H^A, H^B, and between Br^1, Br^2 is:

    (a) H^A, H^B are enantiotropic; and Br^1,$Br^2$are diasterotopic

    (b) H^A, H^B are diastereotopic; and Br^1, $Br^2$are enantiotropic

    (c) H^A, H^B are diastereotopic; and Br^1, $Br^2$are homotopic

    (d) H^A, H^B are enantiotropic; and Br^1, $Br^2$are homotopic**[NET Dec 2012]**

Solution (b) H^A, H^B are diastereotopic; and Br^1, $Br^2$are enantiotropic

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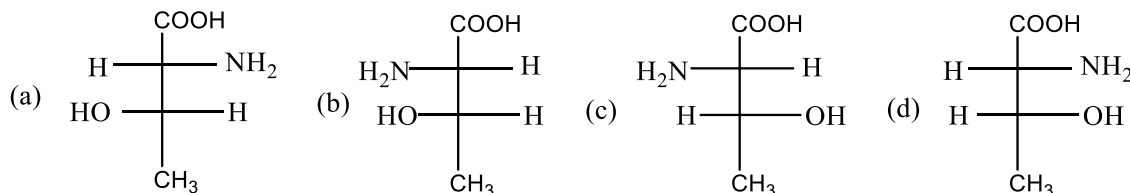**Email**: info@genesis-tutorials.com
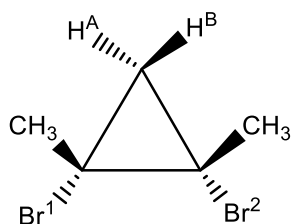
Note:- (i) Homotopic ligands are interchange by C_n axis
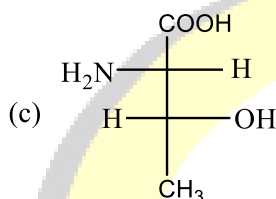
(ii) Enantiotopic ligand are interchange by σ-plane i.e. i and S_n symmetry.

(iii) Diastriotopic ligands are not interchange by any symmetry elements (C_n, i, S_n absent)

Question. The structure of (2S, 3R)-2-amino-3-hydroxy butanoic acid is   **[JAM 2015]**

Solution. (c)

Question. Among the following, the most stable conformation of meso-2,3-dibromobutane is
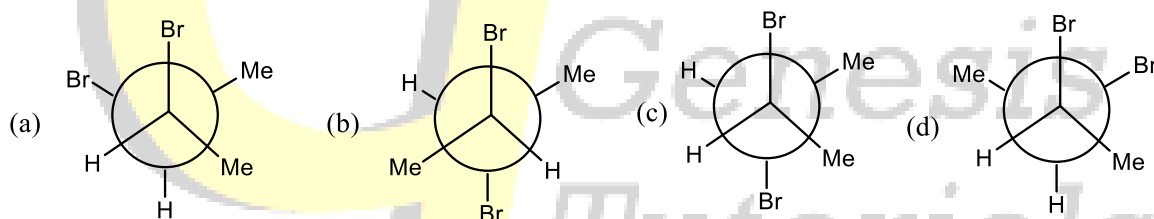
[JAM 2016]

Solution.(b)
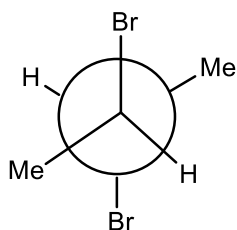
Identical for meso all group shall be anti to each other

Question. Catalytic hydrogenation of the following compound produces saturated hydrocarbon(s). The number of stereoisomer(s) formed is/are   **[JAM 2017]**

(a)   (b) 2   (c) 3   (d) 4

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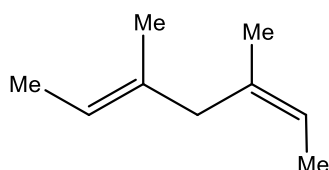
Solution. (c)-3
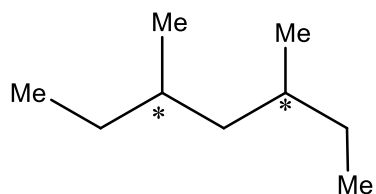
n = number of chiral center

n = 2

number of stereoisomers $= 2^{n-1} + 2^{(n/2)-1}$

$2^{2-1} + 2^{0} = 2 + 1 = 3$

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TOPICITY IN FACES

(1)Homotopic face:-
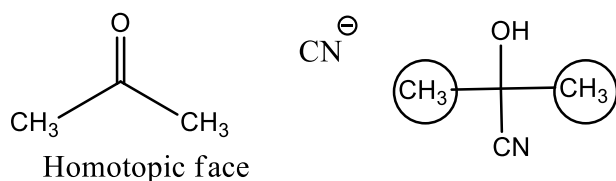
Homotopic face

(2)Enantiotopic face:- Faces of the double bond are said to be enantiotopic if the compound will be achiral and addition on the faces produce enatiomers. Such type of faces is called enantiotopic face.

enantiotopic phase

enantiomers

(having 2 types of altack top & bottom)

enantiotopic phase

+ m-CPBA
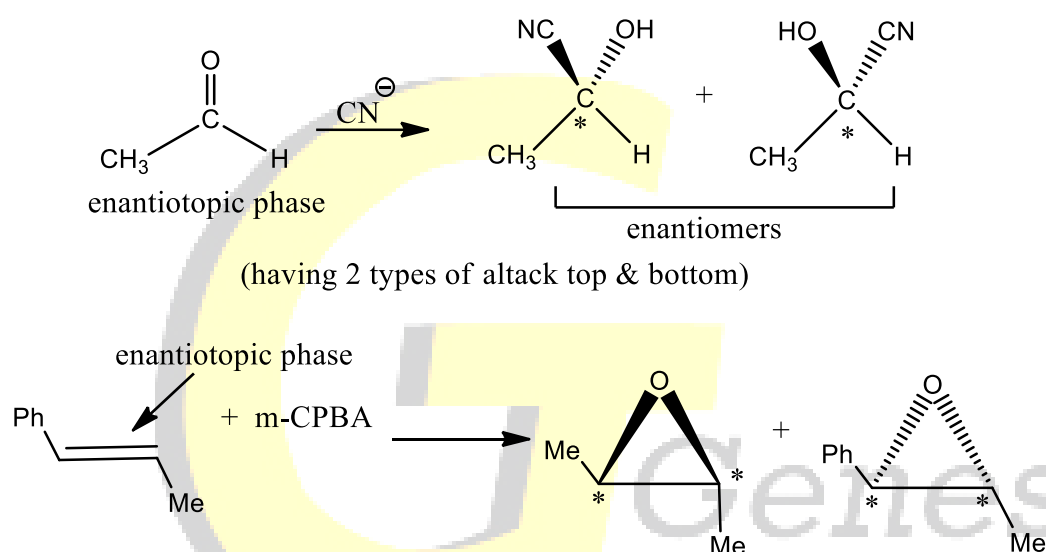
* **Diastereotopic phase**:- Faces of double bonds are said to be diastereotopic if the addition of Nu⁺ in term to form chiral or achiral to produces diastereomeric diasteretopic with each other called diastereotopic faces.

Diastereotopic phase

axial-equitorial →Diastereotopic
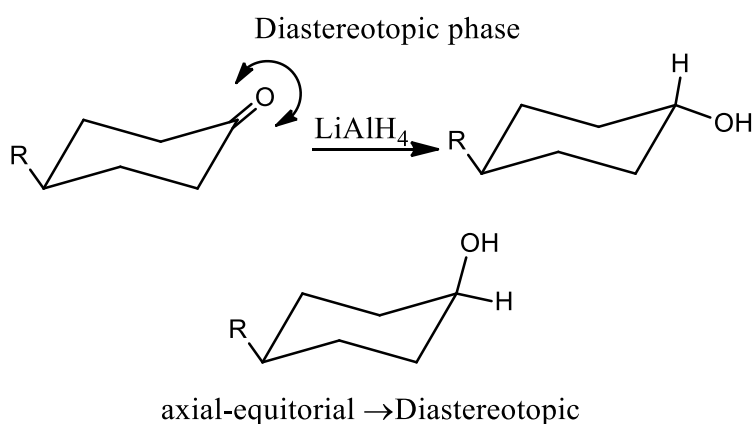
Symmetry:- Disatereotopic are not interchange by C_n $(C_z), S_n$ and i

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Nomenclature of prochiral legands and faces

(1) Prochiral ligands :- (Pro-R & Pro-S)
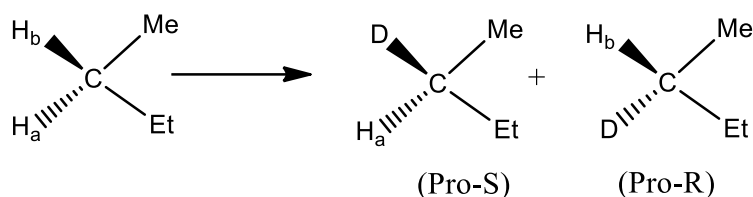

(Pro-S)   (Pro-R)

Note:- (I) For Pro-R & Pro-S configuration newly incoming ligand always give 3rd priority

(II) If incoming ligand priority order is higher than that case substitution takes place by smaller groups like deuterium.

* Nomenclature of phase (Re or Si)

Si-face   Re-face
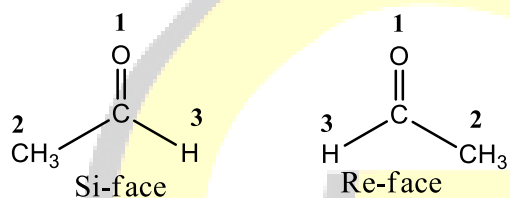
NOTE:- In Re and Si nomenclature, I^{st} priority always gives oxygen and then according

$$\begin{bmatrix} \text{Re For Top site} \\ \text{Si for bottom site} \end{bmatrix}$$

Re   **Si**

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* <u>Calculation of stereoisomers</u>:-
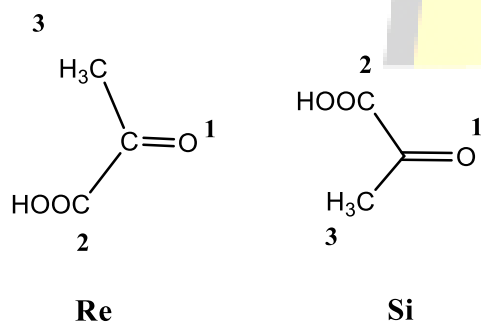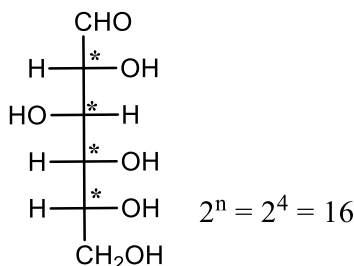
(1) Stereoisomers having n-chiral and have no σ_1, i, S_n in any all possible stereoisomer i.e all stereoisomers are chiral then number of stereoisomers is equal to 2^n
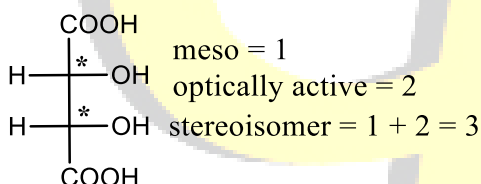
$$
\begin{array}{c}
CHO \\
H \text{---}^* \text{---} OH \\
HO \text{---}^* \text{---} H \\
H \text{---}^* \text{---} OH \\
H \text{---}^* \text{---} OH \qquad 2^n = 2^4 = 16 \\
CH_2OH
\end{array}
$$

(2) Stereoisomer having n-chiral center and have σ plane in at least one of the all possible stereoisomers.

(i) if n = even
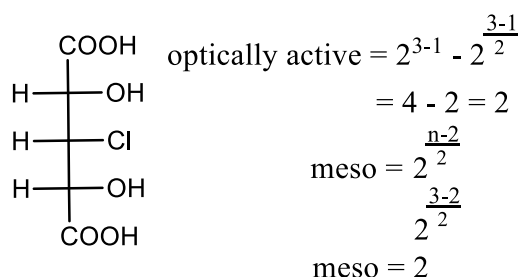
   (i) number of optical isomer = 2^{n-1}

   (ii) number of meso compounds = $2^{\frac{n-2}{2}}$

   Total stereoisomer = optical active + meso

$$
\begin{array}{c}
COOH \\
H \text{---}^* \text{---} OH \\
H \text{---}^* \text{---} OH \\
COOH
\end{array}
\qquad
\begin{array}{l}
\text{meso} = 1 \\
\text{optically active} = 2 \\
\text{stereoisomer} = 1 + 2 = 3
\end{array}
$$

(ii) if n = odd (3,5,7…….)

(Number of meso (optically inactive) $= 2^{\frac{n-1}{2}}$

$$
\begin{array}{c}
COOH \\
H \text{---} OH \\
H \text{---} Cl \\
H \text{---} OH \\
COOH
\end{array}
\qquad
\begin{array}{l}
\text{optically active} = 2^{3-1} - 2^{\frac{3-1}{2}} \\
\qquad = 4 - 2 = 2 \\
\text{meso} = 2^{\frac{n-2}{2}} \\
\qquad 2^{\frac{3-2}{2}} \\
\text{meso} = 2
\end{array}
$$

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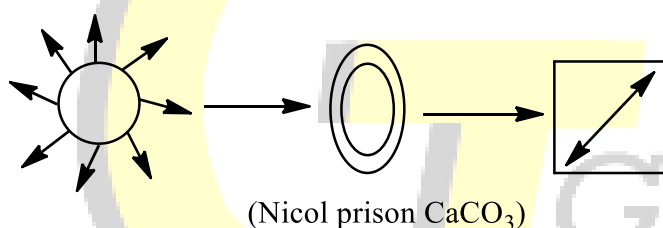**Email**: info@genesis-tutorials.com

<u>Optical behaviour of stereosomers</u>:- The stereoisomers which rotate perpendecular are known as optical isomers and that phenomenon is known optical isomerism

The isomers which rotate perpendicular in clock wise direaction are called dexto (d) or (+) like wise perpendicular rotate anticlock wise are called levol or (-) d and l and isomers or (+) & (-) are enatiomers to each other.

Note:- d/*l* isomers can't be identify not the basis of their configuration it is the polarimetry which help us to identify d/*l* isomers.

CHO
H——OH
CH₂OH
R(+)
glyceraldehyde

CHO
HO——H
CH₂OH
S(-)
glyceraldehyde

* PPL:-

(Nicol prison CaCO₃)
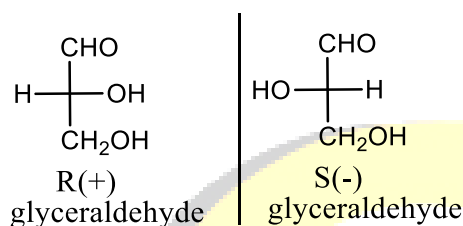
In PPL E.M.R waves oscillate in a single plane perpendicular to the direction of propogation.

* OPTICAL ROTATION (α)

It is the angle of rotation of plane polarized light (PPL) passing through a chiral medium in polarimeter tube is known as optical rotation.

$$\alpha \propto Cl$$

$\alpha = [\alpha]_T^\lambda \, C.l$

$[\alpha]_T^\lambda \rightarrow$ specific rotation

$$\text{temp.} = 20°C, \quad \lambda = 589 \text{ nm}$$

$l = 1\text{dm} \rightarrow 10$ cm

concentration = g/mL or g/cm³

If c = 1gm/cm³ or l = 1dm

$$\boldsymbol{\alpha = [\alpha]_\lambda^T}$$

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SPECIFIC ROTATION:- optical rotation (α) of plane polarized light (PPL) passing through 1 g/mL concentration solution of a chiral molecule in a tube of 1 dm length is known as specific rotation, represented by $[\alpha]_T^\lambda$.

Unit – degree gm^{-1}mL dm^{-1}

Degree gm^{-1} cm^3 dm^{-1}

An optically pure organic compound having molecule unit 200 was analyzed by a measurement of its specific rotation and 2 molar solution of this compound shows +3.5° at 1dm length. Calculate the specific rotation.

Concentration $2M = \frac{2n}{V}$

$= \frac{400}{1000} = \frac{3.5 \times 5}{2 \times 1} = 8.75$ degree gm^{-1} ml dm^{-1}

When 20 miligm organic compound in 1cm^3 tube iof ethanol and solution places in 10 cm long polarizer cell and optical rotation α = -4.35° measured at 20°C with wavelength of 589 nm. Specific rotation of the compound.

20 milligm $= \frac{20}{1000} = \frac{1}{50}$

$C = \frac{\frac{1}{50}}{mL} = C = \frac{1}{50}$

$[\alpha]_\lambda^T = \frac{-4.35 \times 50}{\times .1}$

$[\alpha]_\lambda^T = 217.5$

Optical purity or Enantiomeric excess:-

(i) A solution containing a single enantiomers is said to optically pure or enantiomerically pure.

(ii) A solution containing equal amounts of both enantiomers are said to be optically inactive and called racemization.

(iii) When a solution containing unequal amounts of enantiomers then the form optical purity or enantiomeric excess are used with respect to any enantiomer.

Percentage of d	% of l	Optical purity (ee)
100%	0%	100% w.r.t d
80%	20%	60% w.r.t d
60%	40%	20% w.r.t d
50%	50%	0 w.r.t d
40%	60%	20% w.r.t d
80%	20%	60% w.r.t d

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100%	100%	100% w.r.t d

Optical purity or enantiomers excess

$$ee = \frac{\alpha \text{ mix}}{\alpha \text{ pure}} \times 100\%$$

* %d + % l = 100

$$\boxed{\%d = 100 - \%l}$$

* $\boxed{ee = \frac{[d-l]}{[d+l]} \times 100\%}$

* $\boxed{ee = \frac{R-S}{R+S} \times 100\%}$

* A mixture two enantiomers shows optical rotation + 12°. If the specific rotation is 32° calculate the composition of enantiomers?

Solution α mix = 12°

α pure = 32°

e.e = $\frac{12}{32} \times 100\%$

e.e = + 37.5 (d)

optical purity of d isomer 37.5 %

reci mixture l % = 62.5 %

l % = $\frac{62.5}{2}$ = 31.25%

$$\boxed{l \% = 31.25 \%}$$

31.25 + 37.5

Total d = 68.75 %

Question. (+) Mandelic acid has a specific rotation of +158°. What would be the observed specific rotation of 25% (-)-mandelic acid and 75% (+)-mandelic acid? **[DU 2016]**

(a) +79° (b) 0 (c) −79° (d) +39.5°

$$ee = \frac{\alpha \text{ mix}}{\alpha \text{ pure}} \times 100\%$$

$50 = \frac{\alpha \text{ mix}}{158} \times 100\%$

$= \frac{50 \times 158}{100} = +79°$

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Question. The rotation of pure R(+)-Limonene is +123.0°. Calculate the % of the (+) isomer in a sample showing a rotation of +109°? **[UOH 2011]**

(a) 8.6   (b) 77.2   (c) 94.3   (d) 82.9

$$ee = \frac{\alpha \text{ mix}}{\alpha \text{ pure}} \times 100\%$$

$$ee = \frac{109}{123} \times 100\%$$

ee = 88.6%

This will be obtained by (94.3-5.7 = 88.6). It means that 94.3% (+) isomer and 5.7% of (-_ isomer are present in sample

(c) option

Questionthe specific rotation $[\alpha]_D$ for (S)–(+)–2–butanol is 10° mL/g dm. The observed optical rotation (α_{abs}) of a sample composed of a mixture of (R)- and (S)-2-butanol is -0.45°. If the cell path length is 0.6 dm and the concentration of 2-butanol in the sample is 0.15 g/mL, the percentage of (R) and (S) enantiomers in the sample are **[NET June 2017]**

(a) (R) = 25%, (S) = 75%   (b) (R) = 40%, (S) = 60%

(c) (R) = 60%, (S) = 40%   (d) (R) = 75%, (S) = 25%

Solution$[\alpha] = 10°$ $\alpha_{abs} = -0$

l = 0.6 dm

Concentration = 0.15 g/mL

$[\alpha]_T^\lambda = \frac{\alpha}{Cl}$

$[\alpha]_\lambda^T = \frac{-0.45}{0.6 \times 0.15} = -5°$ $ee = \frac{-5°}{10}$

ee = 0.5 → 50 % with respect to 25% R   25% S

Total (R) = 75%, (S) = 25%**(d)** answer

Question. The $[\alpha]_D$ of a 90% optically pure 2-arylpropanoic acid solution is +135°. On treatment with a base at RT for one hour, $[\alpha]_D$ changed to +120°. The optical purity is reduced to 40% after 3 hours. If so, the optical purity of the solution after 1 hour, and its $[\alpha]_D$ after 3 hours, respectively, would be **[NET Dec 2012]**

(a) 80% and 60°   (b) 70% and 40°

(c) 80% and 90°   (d) 70% and 60°

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Solution: Optical purity also known as ee of a compound of 90% show +135° specific rotations

So, its 100% pure optical isomer will show $= \frac{135}{90} \times 100 = 150°$ specific rotation

At 1 hors the specific rotation reduces to +120°, so the ee or optical purity $= \frac{120}{150} \times 100$

At 3 hours optical purity is 40% So, specific rotation

$\frac{150}{100} \times 40 = 60°$ **Answer**(a) 80% and 60°

optical purity	%d	%l	Specific Rotation
100%	100%	0%	150°
90%	95%	5%	135°
80%	90%	10%	120°
40%	70%	30%	60°

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CYCLOHEXANE

Question The optically active stereoisomer of the following compound is: **[JAM 2011]**
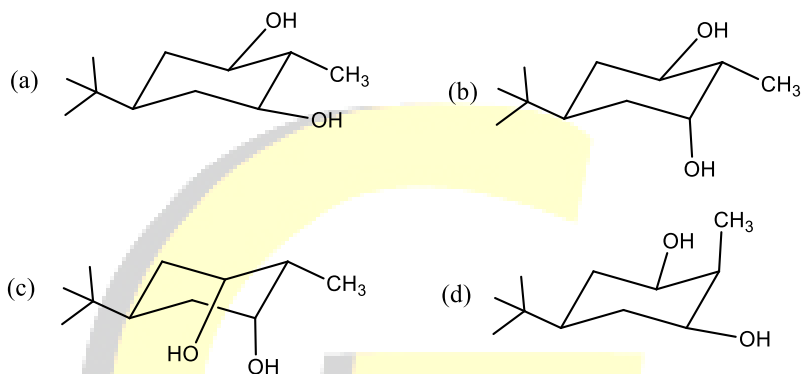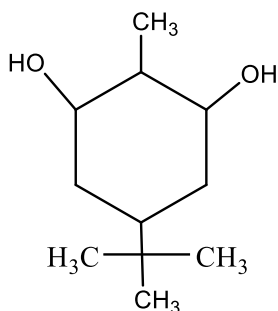
Answer (b)

1,4 position–plane pass, whether it is axial or equatorial
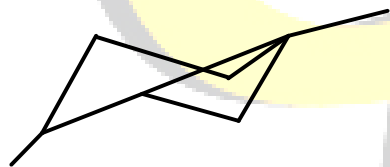
Due to H bond, this configuration is more stable (1,3) position
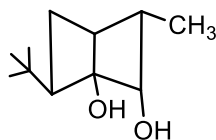
Cyclohexane exists in different form but chair form is most stable form

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Stability order:-

chair form > twist boat form > boat form > half chair
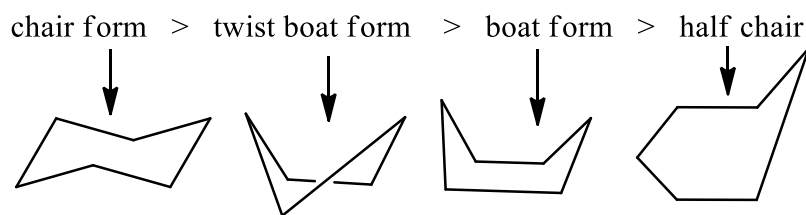
In half chair angular strain is present as well as eclipsing effect is also present that's why half chair is most constable.

In twist boat form eclipsing effect and 1,4-flag pole repulsive, interaction decrease in the twist boat conformation.

NOTE:- Generally in chair form equatorial substituted group cyclohexane is more stable.

95 %   5%
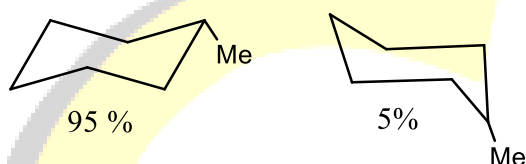
After filing all axial group become equilateral and vice-versa

Question Ring flipping of the compound in the following conformation leads to **[GATE-2016]**

(a)

(b)

(c)

(d)

Solution

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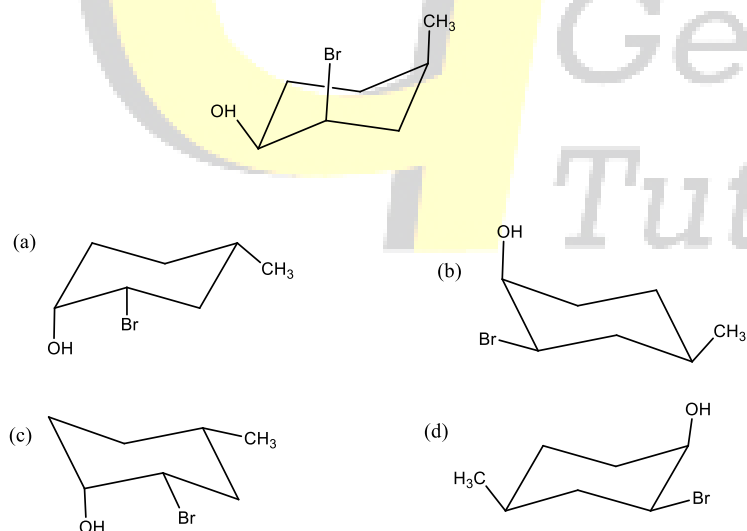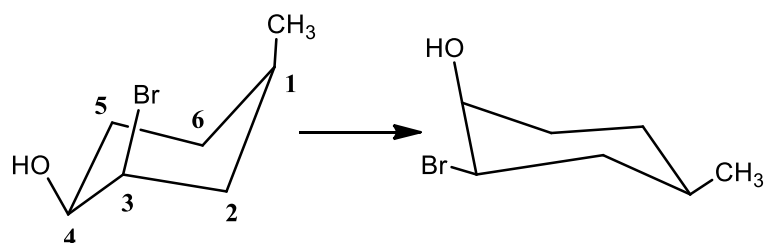
Question:- Bridge-head hydrogen of the conformer of cis-decalin is positioned as **[GATE 2004]**

(a) a, a   (b) e, e   (c) a, e   (d) pseudo-a, pseudo-e

[a = axial; e = equatorial]
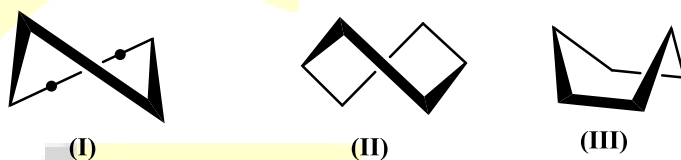
Solution Cis-decaline (2-dot) means (cis)

(a, e⁻)

Answer is (c)

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psedeo-equitorial
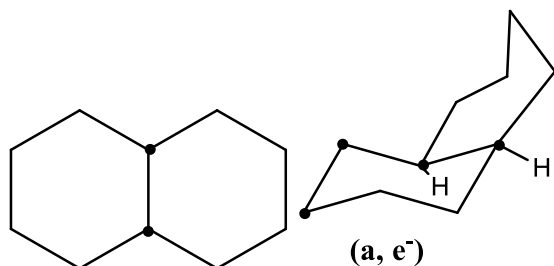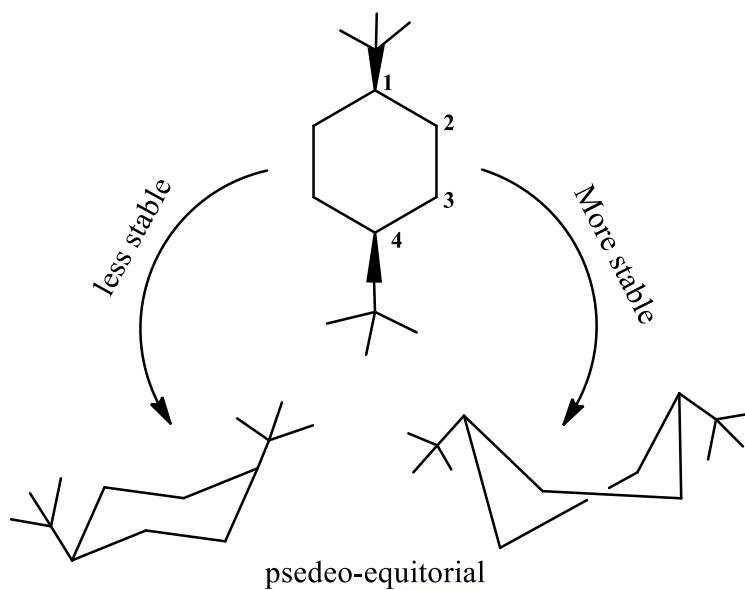
Question. The increasing order of energy of the following conformers is: **[UOH 2016]**

(I)   **(II)**   **(III)**

(a) (II) < (III) < (I)   (b) (I) < (II) < (III)   (c) (III) < (II) < (I)   (d) (I) < (III) < (II)

Solution   (a) (II) < (III) < (I)

I – Half chair

II – Twist boat

III- True Boat

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CYCLOHEXANE DERIVATIVE:-

(more stable boat form due to H-bonds)

Trick **-** above — above
Below — below
Below — above
above — below

less stable

more stable

Cis-1,3-cyclo hexane diol

pseduoequiterial

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*

(I) **(II)** **(III)**

less stable

more stable because interaction between lone pair & t-Bu is not considerable

more stable because interaction between
lone pair & CH$_3$ is not considerable

*

(pipredene) OR

More stable
gauche no interaction

gauche interaction

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More stable

less stable

More stable
Due to space filling model

Ph   Me

≡

Ph

Me

More stable   More gauche interaction

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Question. The configuration at the two srerocentres in the compound given below are
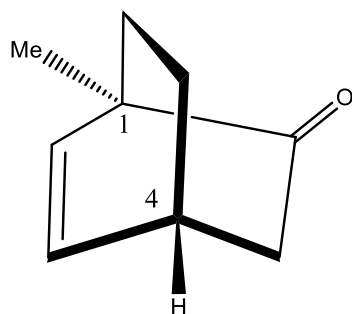
[**NET June 2011**]

(a) 1R, 4R   (b) 1R, 4S   (c) 1S, 4R   (d) 1S, 4S
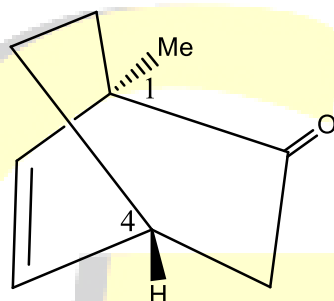
Solution.

Answer is **option (a)**

QuestionThe absolute configuration at the two chiral centres of (–)–camphore is:

[**NET Dec 2012**]

(a) 1R, 4R   (b) 1R, 4S   (c) 1S, 4R   (d) 1S, 4S

Solution

Answer:- (d) 1S, 4S

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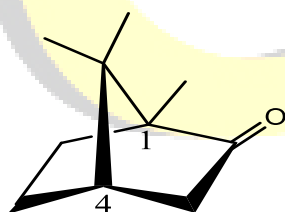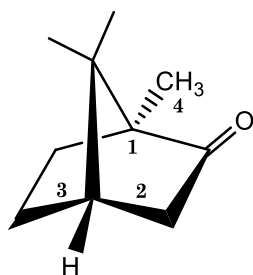
* ANOMERIC EFFECT:-

(i) Presence of the pyranose ring.

(ii) Presence of electronegative group at Anomeric carbon must lies at axial position to give most stable structure/conformer.

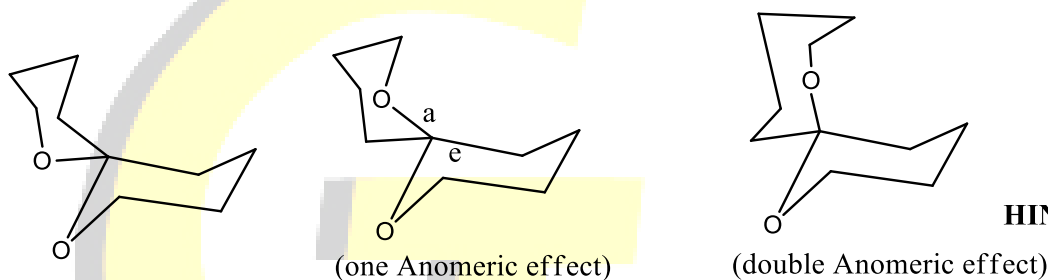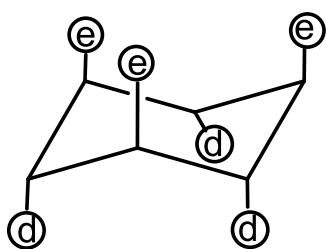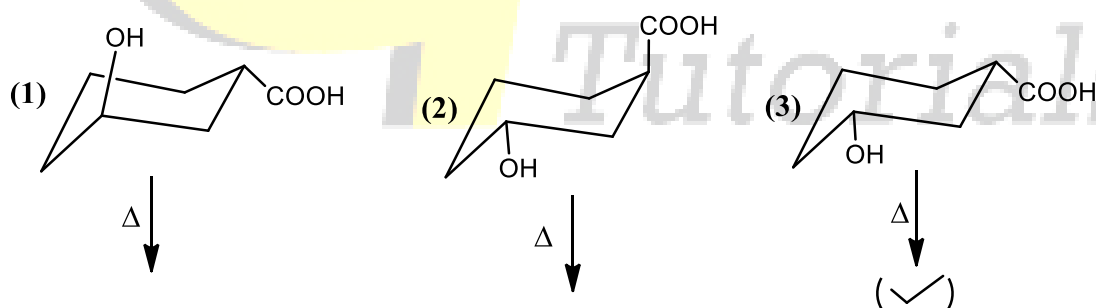Group or Atom X. lipe -OH, -OMe, -COR, -Cl, -Br, NH-R, etc.

More stable

More stable Anomeric effect

(n to α^* transition)
(domination over 1,3 dixaxial interaction & gauche interaction)

n- α^* not possible
(does not show anomeric effect)

σ- π^* tranistion is not possible due to large gap of enegy

SN^1
$Cl^\ominus$

(major due to anomeric effect

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* DIMETHOXY METHANE

Me — O — CH$_2$ — OMe

MeO — C — OMe (with H above and below C)

Most stable form Gauche form
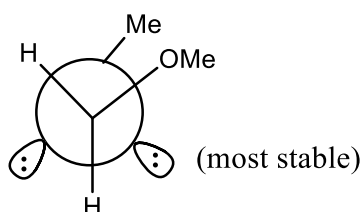
(most stable)

Question:- Which is most stable?

(one Anomeric effect)   (double Anomeric effect)

HINT:- Anomeric Effect

Question:- Which compound form lactones?

(1) OH ... COOH

(2) COOH ... OH

(3) COOH ... OH

Δ

(e) → carbon-elevated carbon

(d) → Carbon- depressed carbon

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(lectene)

*

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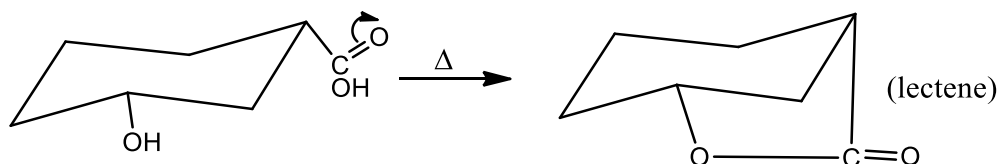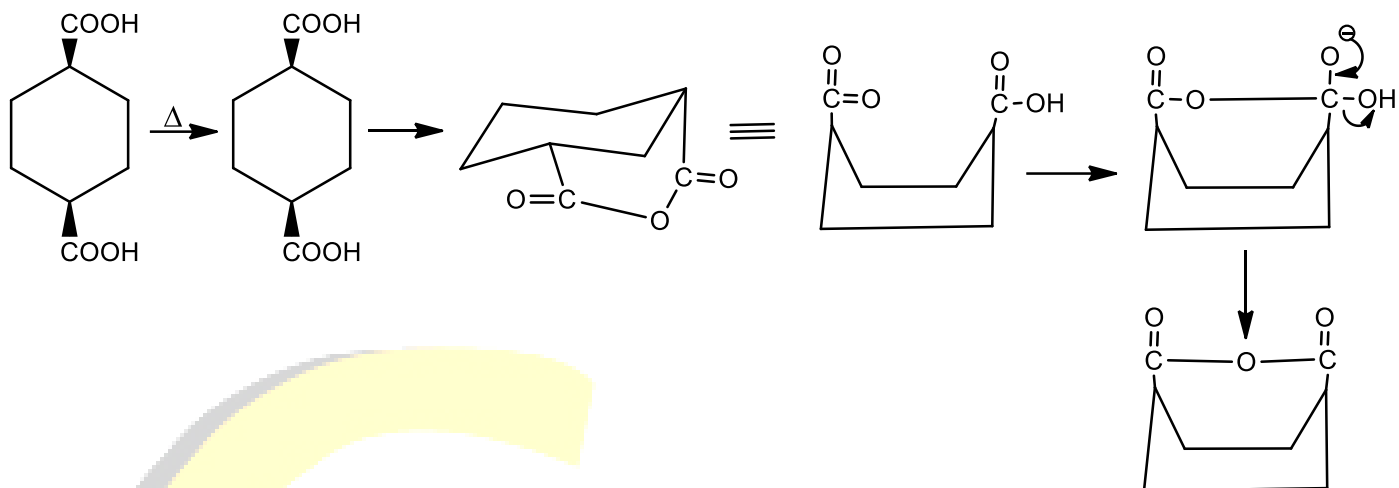
(1) Rate of decarboxylation:-

(a) (More stable)

(b) (less stable)

(c) slow

(d) (fast due tp EWG)

(d) > (c)

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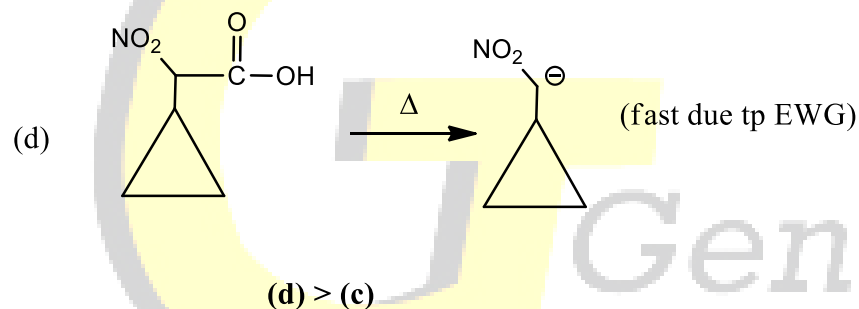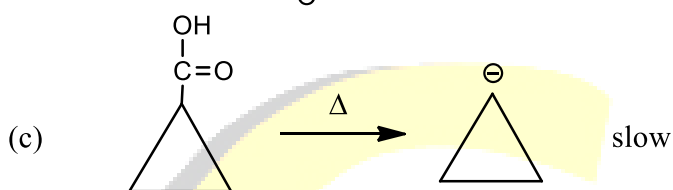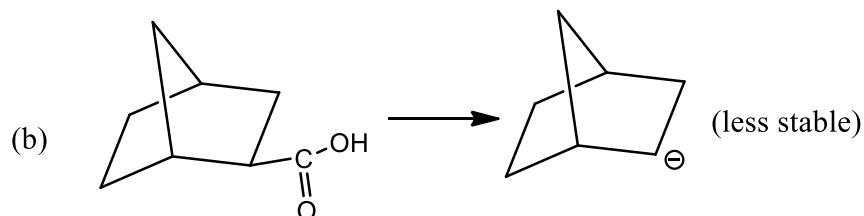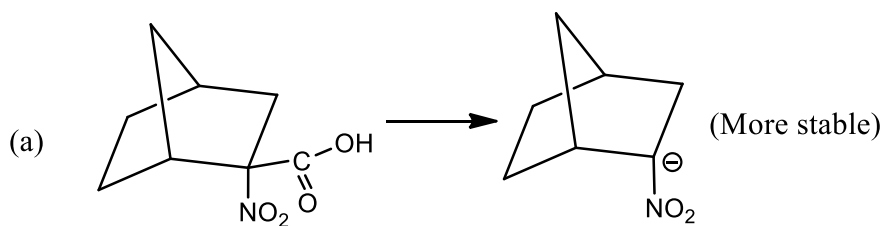
CONFORMATIONAL ANALYSIS:-

If two different 3-D arrangement of a molecule are inter convertible into each other nearly by free rotation about single bond are called conformer.

Conformer cannot be isolated, because they exist in dynamic equilibrium.

* Conversion of one conformer into another depends on energy barrier if the energy barrier is small that can be achieved at ambient temperature conformer remain in a rapid equilibrium.

* If energy barrier for rotation of single bond is very large than one conformer cannot be converted into another such conformer are isolated and also called configuration isomer.

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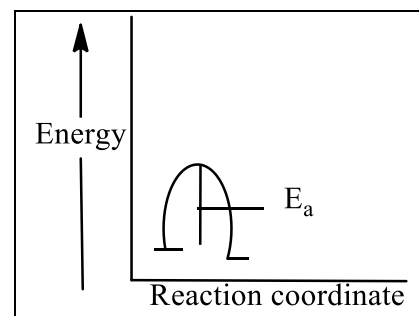
STRAIN IN CONFORMER

(1) Torsional strain:- it is a repulsive force which operates between co-valent e⁻(s) (covalent bond) of two vicinal atoms in eclipsed conformation.
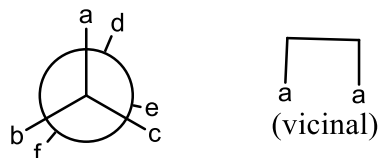
(3-torisonal strain)

* Contribution of each torsional strain in potential energy conformer:-

X	Y	
H	H	1 Kcol/mol
M	Me	1.4
Me	Me	3.4 – 3.6
Et	Et	3.7-3.8

(2) Angle strain:- (Beyer strain):- This type of strain is found in cyclic molecule any deviation form normal sp³ bond-angle 109° 28′

$$d = \frac{1}{2}[109° 28' - \theta]$$

(1) Cyclopropane - $\Delta/ = \frac{1}{2}[109° 28' - 60]$

$$d = 24°44'$$

* Derivation $\propto \frac{1}{stability}$

* Butane Gauche interaction:- Found in staggered conformer between bulkyer groups/ligands separated by approximately 60°
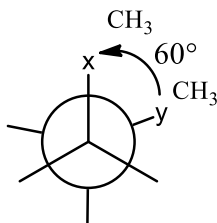
* Contribution of each Gauche interaction in potential energy of a conformer 1,3-diaxial interaction in cyclic compounds:-

X	Y	
H	H	0.00
Me	H	0.00
Me	Me	0.9 Kcol/mol
Et	Et	≤ 0.9 ≈(1) Kcal/mol

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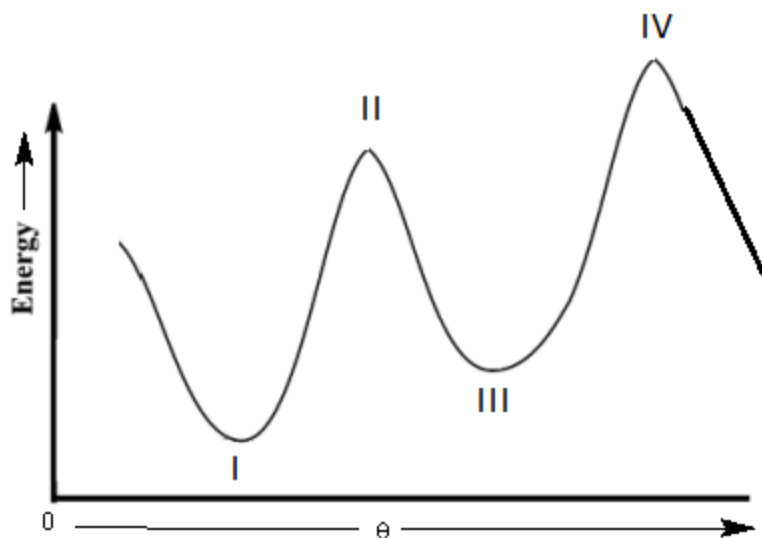* Dihederal Angle:- $[\theta] \rightarrow$ It is defined as angle between two bisecting planes of two bonds present at vicinal carbon atom.

It is non-directional in nature i.e it does not tall anything about the direction of rotation of single bond in conformer

* CONFORMATION OF n-Butane

$CH_3 - CH_2 - CH_2 - CH_3$ n-butane

*NEW MANN PROJECTION FORMULA:-

Potential Energy Diagram for this stability I > III > II > IV

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Question. Given the energy of each gauche butane interaction is 0.9 kcal/mol, ΔG value of the following reaction is **[NET Dec 2012]**
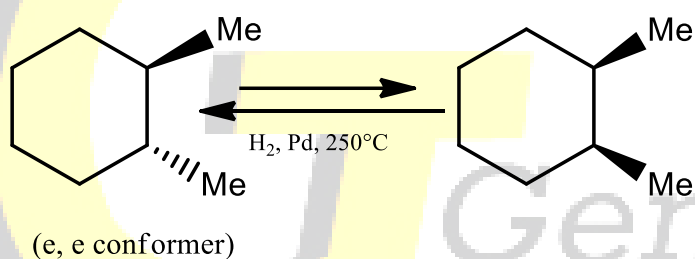
(e, e conformer)

(a) 0.9 kcal/mol   (b) 1.8 kcal/mol (c) 2.7 kcal/mol   (d) 3.6 kcal/mol

Solution

$9 \times 4 = 3.6$ **kcal/mol** $0.9 \times 2 = 1.8$ **kcal/mol**
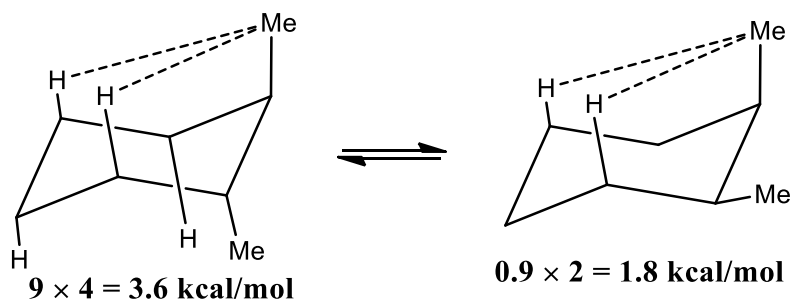
$\Delta G = G_2 - G_1$ free energy (2)

$\Delta G = 3.6 - 1.8$ $\boxed{1.8 \, kcal/mol}$

Question. The gauche conformation ($\varphi = 60°$) of n - butane possesses   **[NET June 2013]**

(a) plane of symmetry; and is achiral   (b) C_2-axis of symmetry: and is chiral

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(c) centre of symmetry; and is achiral   (d) plane of symmetry; and is chiral

Solution.
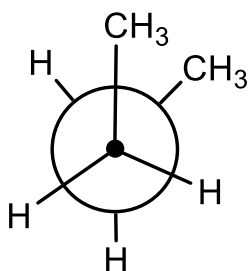
(b) C_2-axis of symmetry: and is chiral

(Gauche form is optical active)
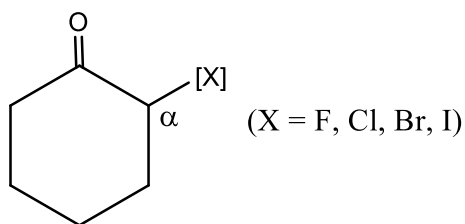
* IN LIQUID PHASE:- (Benzene-solvent)

(52%)   (48%)
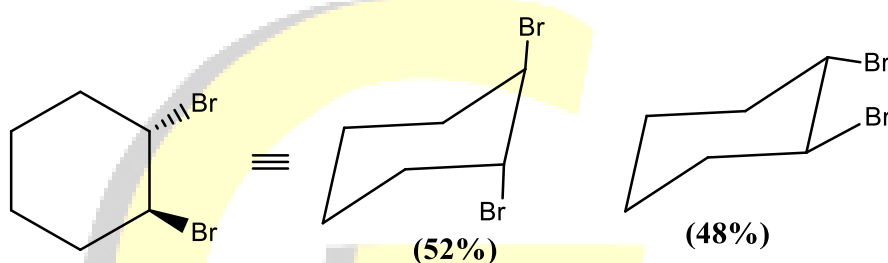
* IN GASEOUS PHASE

(95%)   (5%)
          less stable
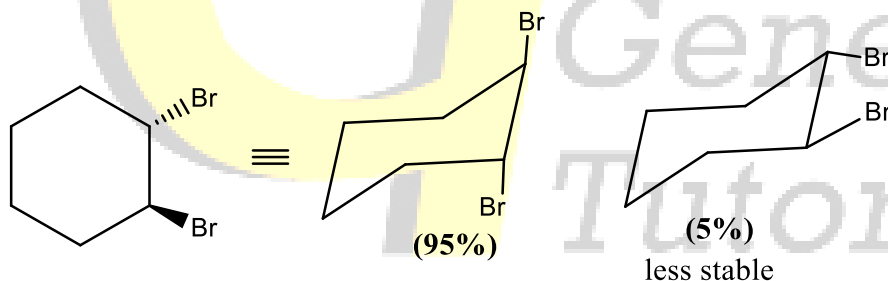
In gaseous phase less stable- due to dipole-dipole interaction

* ∝ −halo ketone effect:-

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(X = F, Cl, Br, I)

less stable

more stable
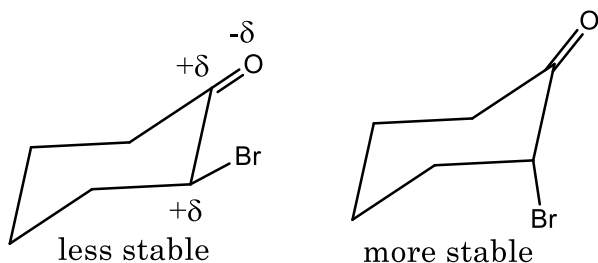
dipole interaction

* **(Interaction → repulsion)**

* <u>**BREDT'S RULE:-**</u> (Bridge head carbon does not have planarity)

● = **(bridging carbon)**

bridege head carbon
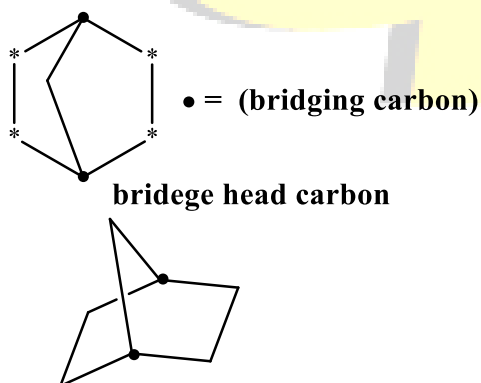
Rule- Bridge head carbon cannot be sp^2 hybridized unless ring size is large enough.

Carbocation/double Bond → not doing exist.

Cause:- Bridgehead and adjacent carbon both are orthogonal to each other that's why proper overlapping not tales place.

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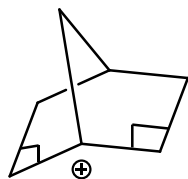
sp^2 120°

strain increase → unstable

Example

stable

not possible
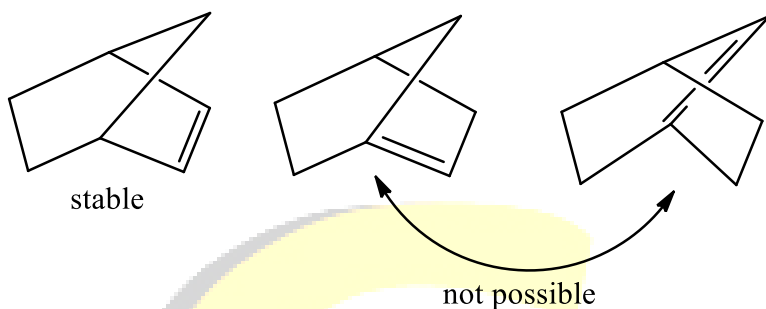
Application:-

(i) Stability of C$^{\oplus}$

(a)

(b)

(c)

6 α-H

2 α-H

6 α-H

(c) > (b) > (a)

(ii) Size of ring

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(I)
5C

(II)
6C

(III)
7C
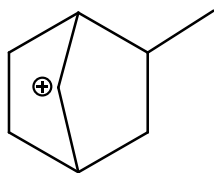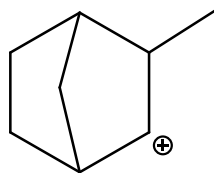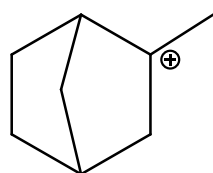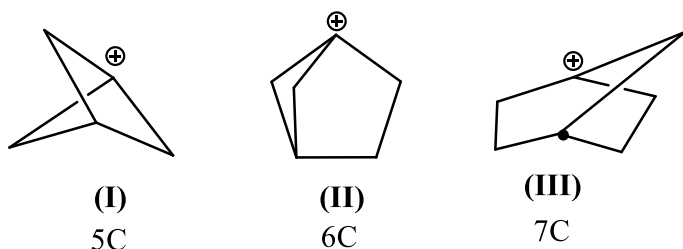
Stability of B.H.C $\overset{\oplus}{}$ depends upon ring size (number of atom in a system)
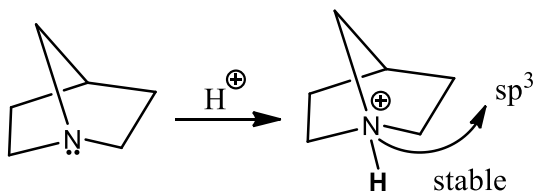
c > b > a

Stability increase
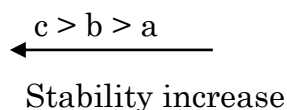
Anti-Bredts Rule:-
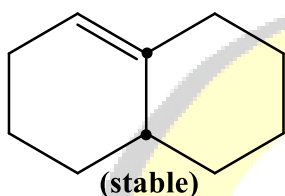
(stable)

Number of bridging carbon = 8

If briding carbon ≥ 8, the compound will be stable

(stable)

stable

sp^3
stable

stable

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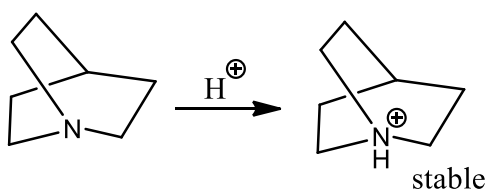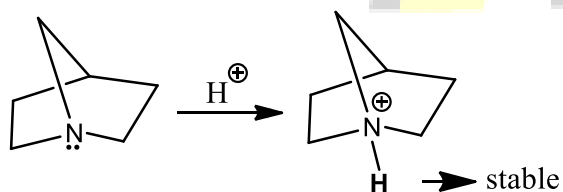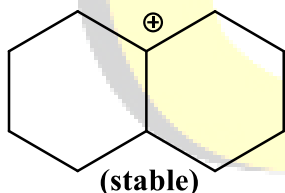
Cram's Rule

* Diastereoselectivity in addition reaction of chiral carbonyl compounds

10%   90%
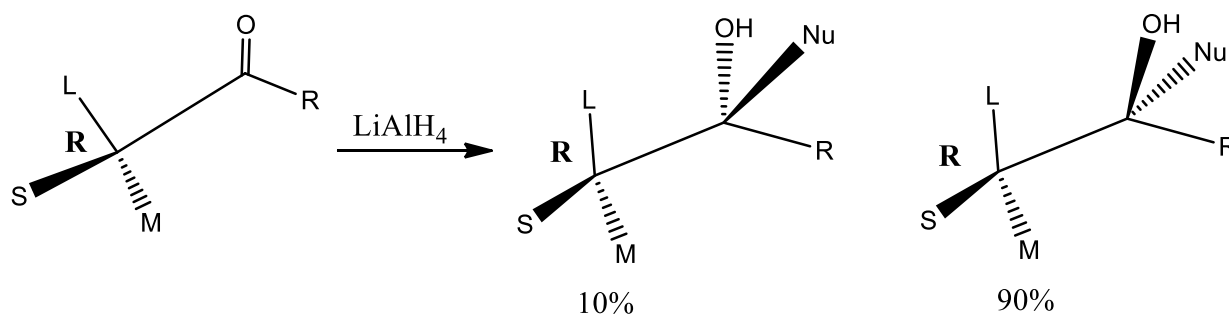
In the addition reaction of carbonyl compounds having chiral center at adjacent carbon distereomeric product which one of the distereomers could be predicted following rules:-

(1) Cram's rule

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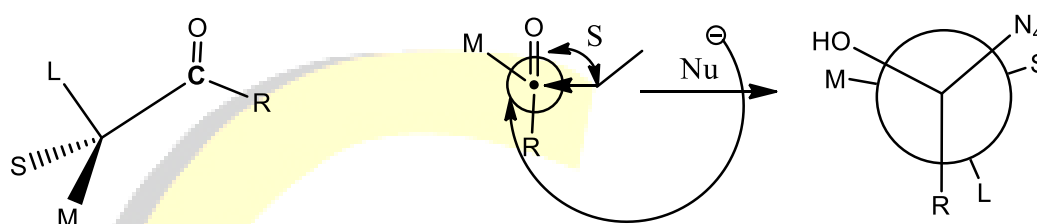**(2)** Dipole cram's Rule

(3) Fekin-Anti model

(4) Rigid cyclic (Chelation model)

(1) Cram's Rule:-

(i) Draw the Newmann projection of chiral carbonyl compounds placing bulkiest (large) anti to carbonyl group

(ii) Allow to nucleophile to attack from side of small group
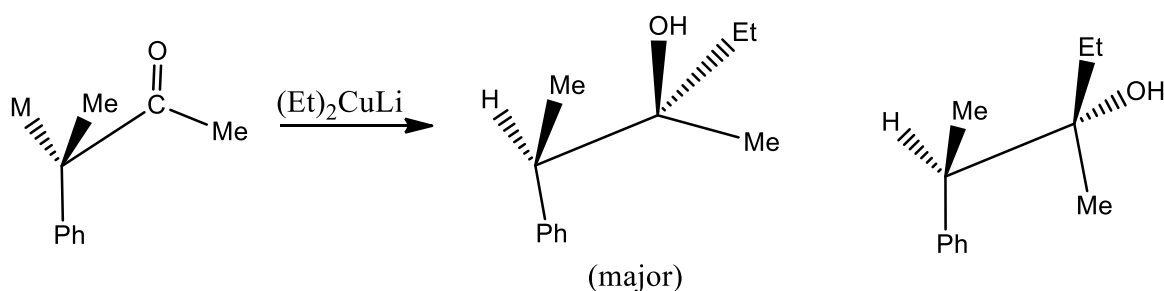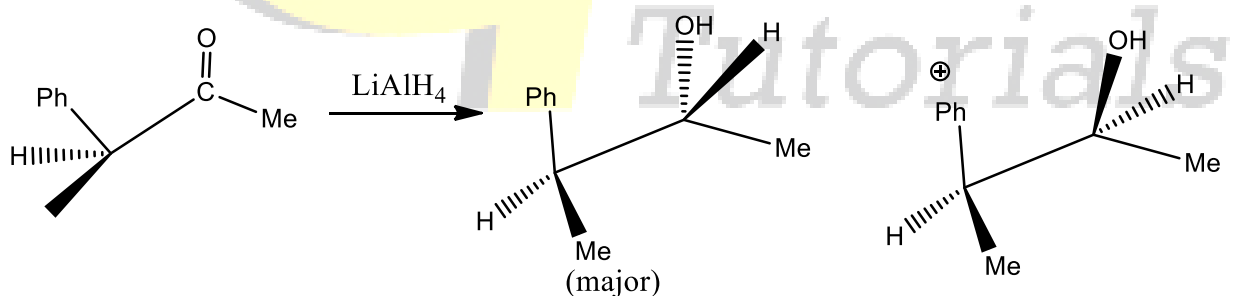
(iii) Re-draw product in zig-zig fashion

B.D angle → Burgle Dainty angle

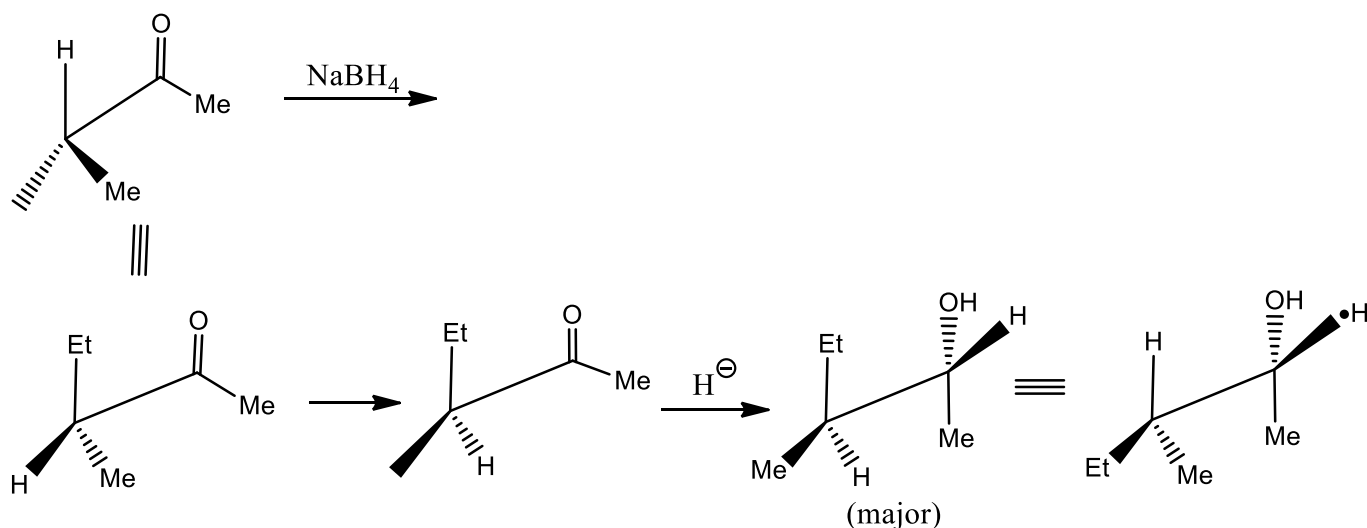**Trick**

If large group Anti (Nu$^{\oplus}$ attack from smaller group side)

If large group syn (Nu$^{\oplus}$ attack from medium group side)

*

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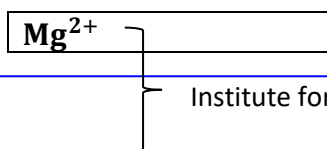**Web**: www.genesis-tutorials.com
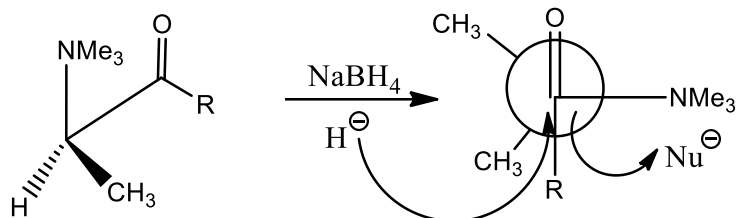**Email**: info@genesis-tutorials.com

DEMERIT'S OF CRAM'S RULE:-

(1) Chiral carbonyl compounds having EWG do not follows cram's such type of reaction can be predicted by dipole cram's rule

(2) If hetroatom like oxygen, Nitrogen, sulpher are present at chiral centre of carbonyl compound cram's rule may be wrong information.

(3) Although cram's rule predict the stereo chemical relation but if fails to explain the Quantitive assessment of asymmetric induction in form of steric interaction.

Felkin-Anti Model:- According to this model the most stable conformation of carbonyl compounds having chiral centre at adjacent atom are those in which the large group/heteroatom non-chelating condition is perpendicular to the carbonyl group.

$\left. \begin{array}{c} Na^+ \\ K^+ \end{array} \right]$ non $-$ chelating $*$/Li^+ often (when O is hetro atom)

$\boxed{Mg^{2+}}$

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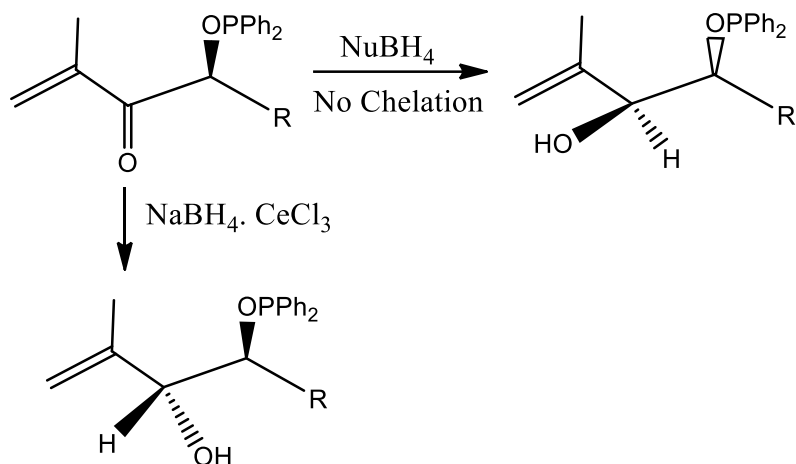$$Zn^{+2} \quad \text{Chelating}$$
$$Ti^{3+}$$

If Reagent having chelating (like Mg^{2+}, Ti^{3+}, Zn^{2+} etc) & carbonyl compound having hetroatom at chiral centre than that condition large group (hetro group) will be perpendicular to carbonyl.
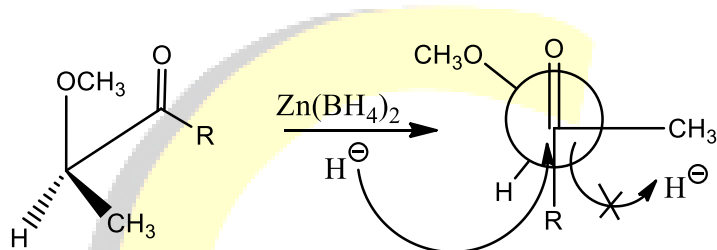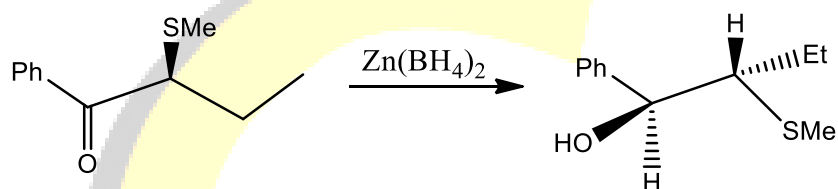

* TRICK → [For chelating]

(*) If large group is parallel to C = O then stereo of incoming group will be same as smaller group stereo.

(*) If large group (hetro atom) is perpendicular to C = O then the, stereo of incoming Nu^+ will be same as medium group stereo.
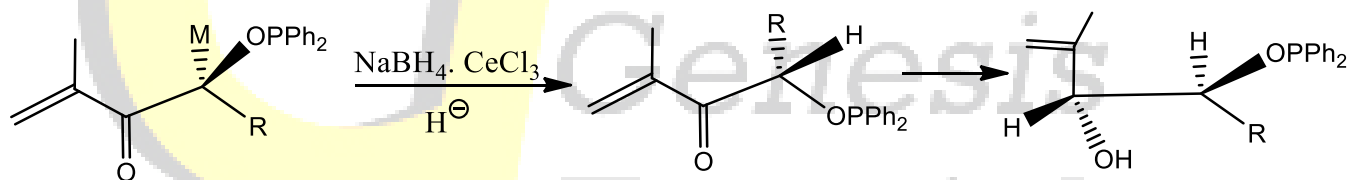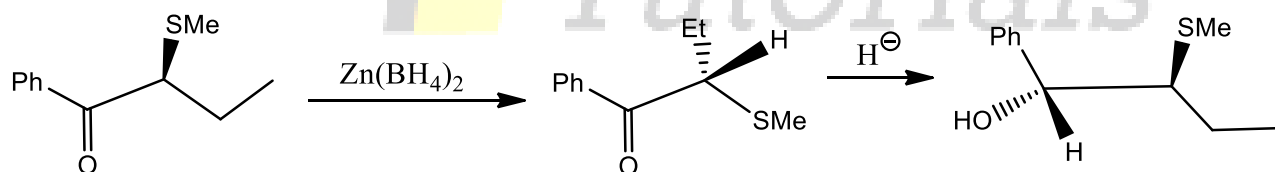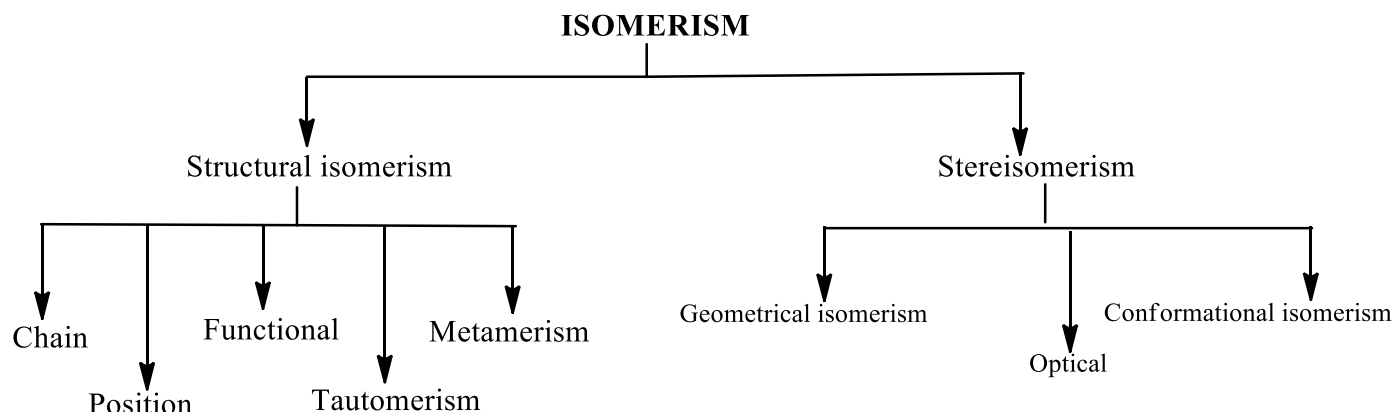
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Major

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(Major)

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ISOMERISM

```
                    ┌──────────────────────────┴──────────────────────────┐
              Structural isomerism                                  Stereisomerism
     ┌────────┬──────┴────┬──────────┐                  ┌──────────────┬──────────────┐
   Chain   Position  Functional  Metamerism      Geometrical isomerism    Conformational isomerism
                        Tautomerism                          Optical
```
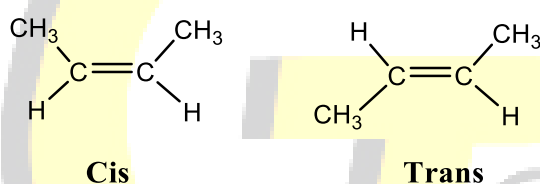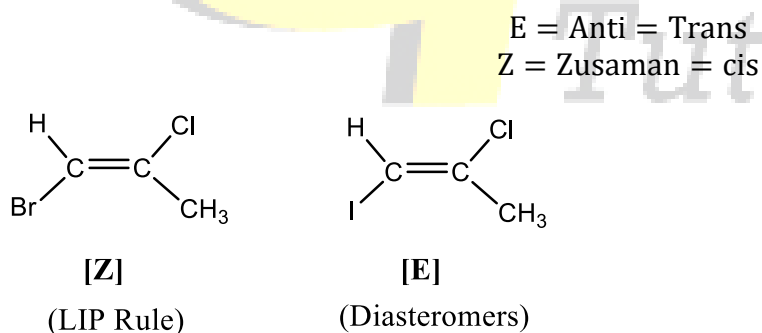
Geometrical Isomerism:- It is also called cis-trans isomerism.

(1) Geometrical isomerism are alway diastereomers

(2) Geometrical isomerism are also a type of stereoismerism

(3) If two same group present in same side then this is called cis and another will be trans.

CH$_3$ CH$_3$ H   CH$_3$
   C = C   C = C
H   H   CH$_3$ H
    Cis   **Trans**

When any alkene having three different group then in that condition cis-trans not applied that type of molecule we introduce E/Z nomenclature
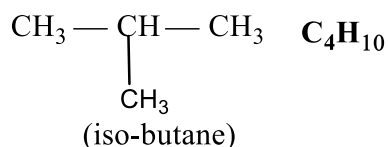
E = Anti = Trans
Z = Zusaman = cis

H   Cl   H   Cl
   C = C   C = C
Br   CH$_3$ I   CH$_3$
   [Z]   **[E]**
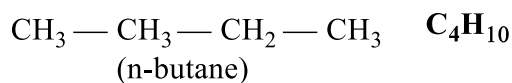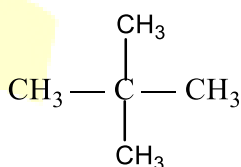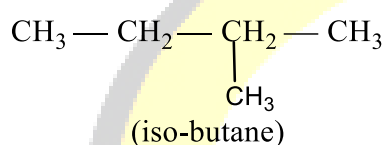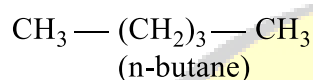(LIP Rule)   (Diasteromers)

STRUCTURAL ISOMERISM:-

The compounds having same molecular formula but different structure that is different arrangement of atoms or group molecule within the molecule are called structural isomers, thephenomenon is called structural isomerism.

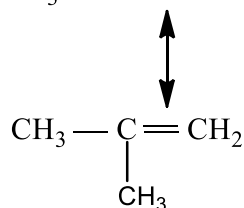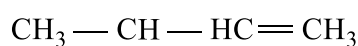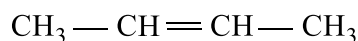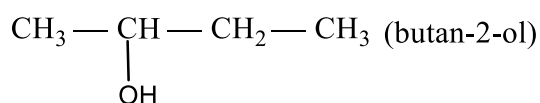Structural isomerism can be divided into following categories.

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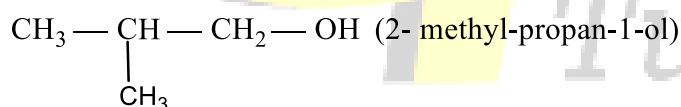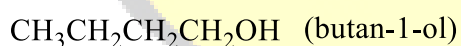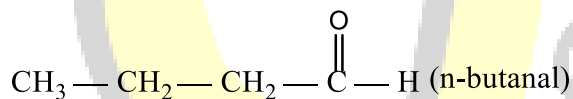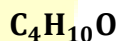**Email**: info@genesis-tutorials.com

Chain isomerism:- The compound having some molecule formula but different arrangement of C-chain (skeleton) with the molecule are called chain isomers, and the phenomenon is called chain isomerism.

$$CH_3 — CH_3 — CH_2 — CH_3 \quad \textbf{C}_4\textbf{H}_{10}$$
(n-butane)

$$CH_3 — \underset{\underset{CH_3}{|}}{CH} — CH_3 \quad \textbf{C}_4\textbf{H}_{10}$$
(iso-butane)

iso-one Me group at second last or second first in chain

$$\textbf{C}_5\textbf{H}_{12}$$

$$CH_3 — (CH_2)_3 — CH_3$$
(n-butane)

$$CH_3 — CH_2 — \underset{\underset{CH_3}{|}}{CH_2} — CH_3$$
(iso-butane)

$$CH_3 — \underset{\underset{CH_3}{|}}{\overset{\overset{CH_3}{|}}{C}} — CH_3$$
Neo-pantane

$$\textbf{C}_4\textbf{H}_{10}\textbf{O}$$

$$CH_3 — CH_2 — CH_2 — \overset{\overset{O}{\|}}{C} — H \ (\text{n-butanal})$$

$$CH_3CH_2CH_2CH_2OH \quad (\text{butan-1-ol})$$

$$CH_3 — \underset{\underset{CH_3}{|}}{CH} — CH_2 — OH \ (\text{2- methyl-propan-1-ol})$$

$$CH_3 — \underset{\underset{OH}{|}}{CH} — CH_2 — CH_3 \ (\text{butan-2-ol})$$

$$\textbf{C}_4\textbf{H}_8$$

$$CH_3 — CH = CH — CH_3$$

$$CH_3 — CH — HC = CH_3$$

$$\updownarrow$$

$$CH_3 — \underset{\underset{CH_3}{|}}{C} = CH_2$$

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Position isomerism:-

Compounds which have same Molecular formula but different in the position of functional groups.

$$C_4H_8 \longrightarrow CH_3—CH=CH—CH_3 \Big/ CH_3—CH—CH=CH_2$$

$$C_3H_7OH \longrightarrow CH_3—CH_2—CH_2—OH \Big/ CH_3—\overset{OH}{CH}—CH_3$$
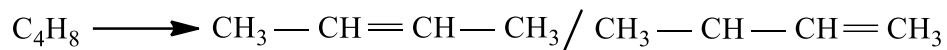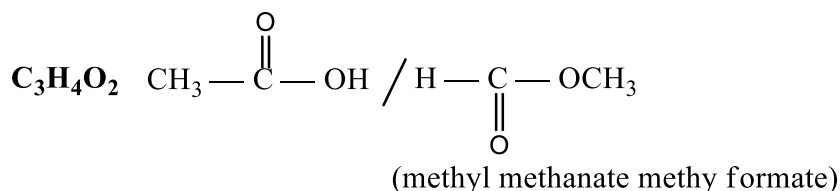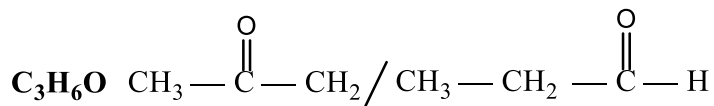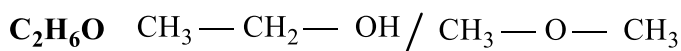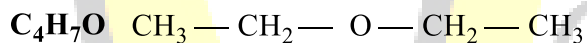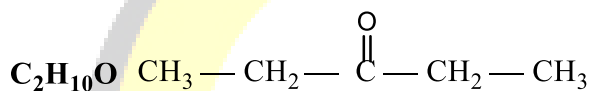

$$C_4H_6 \longrightarrow CH_3—CH_2—C\equiv CH \Big/ CH_3—C\equiv C—CH_3$$

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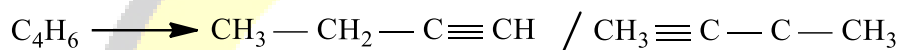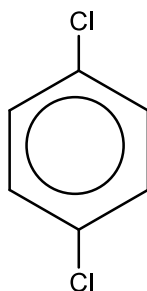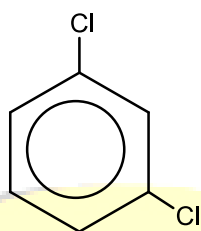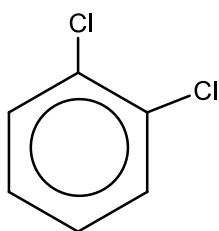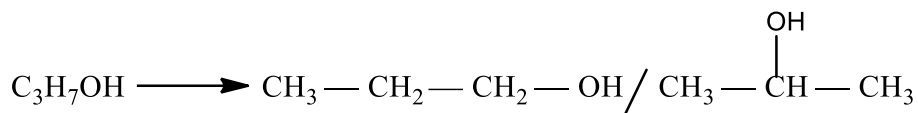
FUNCTION GROUP ISOMERISM

Compound having same molecular formula but different functional groups.

C_2H_6O $CH_3 — CH_2 — OH \Big/ CH_3 — O — CH_3$

C_3H_6O $CH_3 — \overset{\overset{O}{\|}}{C} — CH_2 \Big/ CH_3 — CH_2 — \overset{\overset{O}{\|}}{C} — H$

$C_3H_4O_2$ $CH_3 — \overset{\overset{O}{\|}}{C} — OH \Big/ H — \underset{\underset{O}{\|}}{C} — OCH_3$
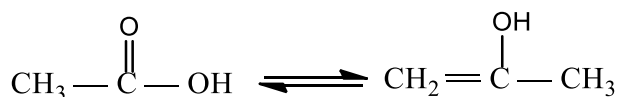
(methyl methanate methy formate)

METAMERISM

The compound having same molecular formula but different number of carbon atoms or alkyl group on either side of the functional group are called metamers

$C_2H_{10}O$ $CH_3 — CH_2 — \overset{\overset{O}{\|}}{C} — CH_2 — CH_3$

$CH_3 — CH_2 — CH_2 — \overset{\overset{O}{\|}}{C} — CH_3$

C_4H_7O $CH_3 — CH_2 — O — CH_2 — CH_3$

$CH_3 — O — CH_2 — CH_2 — CH_3$

TAUTOMERS:-

This is a special type of functional isomerism in which the isomers differ in the arrangement of atoms but they exist in dynamic equilibrium which each other.

(1)

$CH_3 — \overset{\overset{O}{\|}}{C} — OH \rightleftharpoons CH_2 = \overset{\overset{OH}{|}}{C} — CH_3$

(2)

$CH_3 — \underset{\underset{O}{\|}}{C} — CH_2 — \underset{\underset{O}{\|}}{C} — CH_3 \rightleftharpoons CH_3 — \overset{\overset{O}{\|}}{C} — CH = \overset{\overset{OH}{|}}{C} — CH_3$

H-bonding

Keto-enol isomerism